Molecular dynamics beyond the limits: massive scaling on 72 racks of a BlueGene/P and supercooled glass transition of a 1 billion particles system

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Abstract

We report scaling results on the world’s largest supercomputer of our recently developed Billions-Body Molecular Dynamics (BBMD) package, which was especially designed for massively parallel simulations of the atomic dynamics in structural glasses and amorphous materials. The code was able to scale up to 72 racks of an IBM BlueGene/P, with a measured 89% efficiency for a system with 100 billion particles. The code speed, with less than 0.14 seconds per iteration in the case of 1 billion particles, paves the way to the study of billion-body structural glasses with a resolution increase of two orders of magnitude with respect to the largest simulation ever reported. We demonstrate the effectiveness of our code by studying the liquid-glass transition of an exceptionally large system made by a binary mixture of 1 billion particles.

Keywords:
supercooled liquids, large scale parallel computing, molecular dynamics, thermodynamics of glasses

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1. Introduction

Recently, contributing to the 2009 annual survey of the EDGE foundation entitled "What will change everything" [2], T. Sejnowski foresees that the computers will be the "microscopes of the future" and, specifically, that are computers that "have made it possible to localize single molecules with nanometer precision and image the extraordinary complex molecular organization inside cells". In his contribution Sejnowski was recognizing the importance of automatic and computerized control of laser beam and image analysis in modern optical microscopy. However, more importantly, computers can be also considered as "future microscopes" for the capability of simulating at the atomic scale the behavior of matter and biological systems. To reach this goal, which was even unthinkable up to some decades ago, it is necessary to develop software able to simulate the newtonian dynamics of a large number of atoms (order $10^{12}$, the "number" of atoms in a cell) for long enough time (order microsecond, or $10^{10}$ time steps) [3, 4, 5]. The state-of-the art supercomputers, on the hardware side, and the parallel simulation codes, on the software one, are nowadays on the way to get this result. However, before facing the ultimate problem of simulating the complexity of life (micro-)organisms, one should validate and optimize codes that simulate hard (physical and chemical) systems. Even if smaller than a micro-organism, these systems encompass problems which are extremely demanding in terms of computational resources, with e.g., simulation boxes containing pico-molar quantity of matter and with characteristic times of 0.1 microseconds. Molecular Dynamics (MD) [3] is expected to be the key to efficiently solve these type of problems. As each generation of computers is introduced, in fact, larger and longer simulations are allowed to be run, thus producing better results which answer a variety of new scientific questions. The latest generation of terascale and petascale supercomputers (see e.g., [6, 7, 8]), in particular, holds the promise to enable the development of more realistic and complex interactions, as well as the study of systems made by a very large number ($\approx 10^{10}$) of particles. In the most common paradigm used today, called massively parallel processing, the typical size of computer clusters ranges from several thousand to hundreds of thousands of processing core units. In these architectures, a high degree of parallelization is essential to efficiently utilize the computational power available. While in principle a high level parallelization strategy works fine for small to medium size supercomputer clusters, tuning for specific architectures can be the key to achieve huge scaling performance. The design concepts of today’s processors, in fact, are markedly different from one system to another, and it is necessary to prepare codes having specific architectures in mind in order to optimize both the speed and the bandwidth of memory access, which is typically slow if compared to the processor’s frequency.

With reference to molecular dynamics, several methods have been published in the past which incorporate different degrees of parallelism [3]. To date, MD scaling has been demonstrated up to ten thousand of cores, with a speed of about 7 iterations per second for an ensemble of 1 billion particles running on 65536 cores of a BlueGene/L [8]. For several applications of molecular dynamics,
such as the study of structural glasses \cite{10} where a typical simulation requires $10^{6-7}$ time steps, this speedup is still too small to perform practical calculations. In the study of glasses, and in the more general area of amorphous materials, molecular dynamics simulations are extremely important as they are able to glimpse the system dynamics at spatial scales between $1 - 100$ nm, a range that is completely inaccessible with experimental apparatus \cite{11,12}. However, due to such speed bottleneck problems, present MD studies on glass have been limited to a number of particles (10 million \cite{13}) unable to have simulation boxes large enough to capture the interesting phenomenology at the micron-scale. Therefore, if on one hand it is necessary to improve the scaling of general MD codes at least two orders of magnitude, in order to effectively use the computing power available, on the other it is also important to focus on specific research fields, such as the context of amorphous materials, which are now asking for new levels of performances.

In this article we report the results of our recently developed Billions Body Molecular Dynamics (BBMD) package, and demonstrate its effectiveness in the study (as case study) of structural glasses by analyzing the glass formation of an exceptionally-large particles system. The BBMD code was able to scale on the whole 294912 cores of the BlueGene/P system at the Jülich Supercomputing Centre, which constitutes the world’s largest supercomputer available characterized by 72 racks of an IBM BlueGene/P. In such an extreme scaling test, the BBMD code showed an efficiency of about 90%, and an overall speed of 2 seconds x iteration with 100 billion particles. These results pave the way to the study of very large systems. In order to demonstrate the applicability of our code to the field of amorphous materials, we performed a controlled temperature MD simulation of a system made by 1 billion particles, and studied the supercooled dynamics of the liquid state by varying the temperature in the range $T \in [2, 10^{-4}]$. This simulation has been performed on the Shaheen supercomputer, hosted at KAUST University and constituted by 16 racks of an IBM BlueGene/P. This paper is organized as follows. We begin our analysis by discussing the structure of the BBMD code (Sec. 2), reviewing both parallelizations and optimization strategies. In Sec. 3 we describe BBMD scaling results obtained at the Jülich supercomputing center. We report the code speedup for molecular systems of different size, ranging from 1 billion to 100 billion particles. Communication workload versus calculation execution time is also studied. In Sec. 4 finally, we investigate the glassy dynamics of a 1 billion particles system made by a binary mixture of soft-spheres.

2. The BBMD code

The BBMD code is a highly optimized, parallel C++ MD code for Lennard-Jones particles systems, designed to scale on machines characterized by hundreds of thousands of processors, such as the latest generation of IBM BlueGene/P supercomputers. Much effort was taken to balance design simplicity and code speed, while optimizing at the same time both memory requirements and cache efficiency. In the following, we briefly describe the main structure of the code.
2.1. Interaction potential

BBMD is originally designed to support two main classes of short range interaction potentials:

- The Lennard-Jones potential
  \[ V(r_{ij}) = 4\epsilon_{\alpha\beta} \left( \left( \frac{\sigma_{\alpha\beta}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{\alpha\beta}}{r_{ij}} \right)^{6} \right) \]  
  \[ (1) \]

- The soft-sphere potential
  \[ V(r_{ij}) = 4\epsilon_{\alpha\beta} \left( \frac{\sigma_{\alpha\beta}}{r_{ij}} \right)^{12} \]  
  \[ (2) \]

being \( \sigma \) and \( \epsilon \) two tensors that parametrize the potentials, and \( r_{ij} \) the distance between particles \( i, j \) of species \( \alpha \) and \( \beta \), respectively. Since Eqs. (1)-(2) converge rapidly to zero beyond \( r_{ij} \approx ||\sigma|| \), it is wasteful to consider an interaction between two particles at a long distance. A standard choice in MD is therefore to truncate the potentials beyond the distance \( r_c \), in order to increase calculation’s speed. To avoid any problem due to the discontinuity of \( V(r) \) at \( r = r_c \), we replace Eqs. (1)-(2) with the following potential:

\[ V^*(r) = \left[ V(r) - V(r_c) - (r - r_c) \frac{dV(r)}{dr} |_{r=r_c} \right] \left[ 1 - \Theta(r_c) \right] \]  
\[ (3) \]

with \( \Theta(x) \) being the Heaviside function. The modification (3) applies across the entire interaction range, and the overall spatial domain is decomposed into MD cubic cells of \( r_c \times r_c \times r_c \) volume (Fig. 1).
2.2. Grid-search method

To perform the time evolution of the system, forces between particles have to be calculated and particle pairs whose distance is below the cutoff range $r_c$ have to be found. For this task, we adopt an $O(N)$ linked-list method, with an inexclusive grid that allows more than one particle to occupy a single cell. Newton’s third law is then applied in order to halve the number of neighbors to be checked in the calculation of the forces. In order to guarantee optimal memory efficiency, we developed a bidirectional list structure that contains all the information of the particles: position $x$, velocity $v$, acceleration $a$, mass $m$ and species index $s$ (Fig. 1). The double pointer mechanism allowed an efficient implementation of memory-related operations (e.g., movement of a particles on a different cell or on a different processor) without deleting or creating memory locations but just by moving pointers, which is very fast. Another advantage of such memory structure is that it automatically links together particles which are close in space, thus improving speed efficiency in all search operations. To maintain memory requirement as low as possible, we do not employ any bookkeeping method, such as the neighboring particle list, which are too memory demanding for billion sized particle systems.

2.3. Parallelization

2.3.1. Parallelization scheme

BBMD has been parallelized with the domain decomposition strategy, also known as spatial decomposition, where the simulation box is divided into subdomains and each domain is assigned to each processor (Fig. 1). The Message Passing Interface (MPI) standard is then employed to handle all parallel communications among processes. This type of parallelization has the advantage to require only nearest-neighbor communications, with a few limited global collective operations, and it is therefore well suited for very large supercomputer clusters such as the IBM BlueGene series.

2.3.2. Parallel force calculation

BBMD employs the velocity-verlet time marching algorithm, which is a standard in MD algorithms due to its robustness and accuracy in maintaining conserved quantities, such as the energy and the momentum. In this evolution scheme, the hot spot of the algorithm is the computation of the forces exerted among particles. To perform this calculation, two parallel operations are required: (i) moving particles that stray from the originally associated process and (ii) exchanging particles that belong to borders crossing different processors. In BBMD, particular care has been taken in the design of (i) and (ii) in order to overlap communications and calculations to the maximum extent possible, while optimizing speed and cache efficiency. More specifically, the parallel communication starts with the operation (i) and then proceeds with (ii). In both steps, a one dimensional array containing particles properties (i.e., $x$, $v$, $a$, $m$, $s$) needs to be constructed, and the number of particles to be sent to neighboring processors has to be calculated. In BBMD, these two operations are
overlapped with send/recv MPI communication routines in order to minimize communication time with respect to calculation. The task (i) begins by tagging all the particles that belong to different processors, and sorting them on-the-fly thus minimizing access times in subsequent MPI communications. This is done by exploiting the bidirectional nature of the particle list. In particular, each particle that needs to be sent to a different process is first moved on the tail of its cell list with an $O(1)$ operation, and then tagged by inverting its mass sign. Such tagging procedure avoids the use of an external index and increases the memory efficiency of the code. Besides that, this method automatically groups tagged particles together, and allows to access them sequentially with $O(1)$ operations when MPI send/recv communications are performed. Once the task (i) has been completed, the exchanging of the nearest-neighbor is done with the standard ghost-cell approach [4]. In both (i) and (ii) tasks, one single MPI process is required to communicate with his 26 neighbors. Although being characterized by nearest neighbors communication only, a naïve implementation of this algorithm requires 26 different communications and results in poor scaling performances when a large number of processor is employed. However, by taking advantage of the domain decomposition strategy employed in BBMD, it is possible to reduce the number of total communications to just 6. This is achieved by properly enlarging the communication window, and in particular by exchanging part of the ghost cells during each MPI communication (see e.g., [4] for more details).
2.3.3. BlueGene specific optimizations

In the calculation of the \( \text{sqrt} \) function, required by the computation of Eq. (3), we employ the square root reciprocal BlueGene function \text{frsqrte}, coupled with two Newton-Rapson iterations. More specifically, we replaced the code segment:

\[
\text{rij} = \text{sqrt}(\text{r2});
\]

with:

\[
\text{rij} = \text{frsqrte}(\text{r2});
\]
\[
\text{rij} = ((0.5 * \text{rij}) \ast (3.0 - \text{r2} \ast (\text{rij} \ast \text{rij})));
\]
\[
\text{rij} = ((0.5 * \text{rij}) \ast (3.0 - \text{r2} \ast (\text{rij} \ast \text{rij})));
\]
\[
\text{rij} = \text{rij} \ast \text{r2};
\]

This optimization results in a speed increment of about 7%.

3. BBMD scaling results

The evaluation of BBMD code performances has been carried out on the Jugene system at the J"ulich Supercomputing Center [8], which is composed of 294912 cores (or 72 racks) of an IBM BlueGene/P with total peak performance of 1 PFlops. The test suite consisted of a series of canonical molecular dynamics simulations of a 20 : 80 binary mixture of soft-spheres with the following parameters (here all the units are to be intended as normalized MD units [5]): \( m_i = 1, \sigma_{11} = 1, \sigma_{12} = 0.8, \sigma_{22} = 0.88, \epsilon_{11} = 1, \epsilon_{12} = 1.5, \epsilon_{22} = 0.5 \). In the canonical evolution, the temperature \( T \) has been fixed to \( T = 0.5 \), and the density \( \rho \) to \( \rho = 1.2 \) in order to maintain the system in the liquid state with all the particles randomly fluctuating among different processors. Figure 2 displays BBMD strong scaling results for systems characterized by 1, 10 and 100 billion particles. Although the memory footprint of BBMD permits the number of particles to be increased by up to two orders of magnitude, we concentrated on a range where the code speed was sufficiently fast to implement realistic calculations. In the smallest case of a system with 1 billion of particles, BBMD was able to scale well beyond 10 racks and obtained and efficiency of 68% on 16 racks when compared to a single rack. When the number of particles was increased from 1 billion to 10 billion, 70% of efficiency was achieved between 1 rack and 64 racks. This number was improved even further for systems containing 100 billion particles. In this configuration, BBMD reached an efficiency of 89% on 72 racks (or 294912 cores) when compared to 8 racks.

To investigate the weak scaling performances of the code, we perform a series of runs with a fixed number of cores and with system sizes varying between \( N = 1 \) billion and \( N = 100 \) billion. Figure 3 shows the result of such analysis. When the particles are increased up to three orders of magnitude, the BBMD code shows a perfect linear \( O(N) \) complexity. The improved scaling is due to the proportion of computation with respect to communication time, which appreciably increases when the number of particles grow (Fig. 4).
Figure 3: BBMD weak scaling results: code speed versus number of particles.

Figure 4: BBMD computation versus communication workload for system with increasing particles number N. The measurements have been performed with simulations of 1000 time steps on 16 racks.
As seen in Fig. 4, the communication impact over computation is practically negligible and the overall execution time is dominated by calculations. This is not only the result of the three dimensional spatial domain decomposition employed, which significantly reduces the volume of each MPI process and the number of elements to be exchanged during each iteration, but also relies on the specific overlapping strategy used in the parallel calculation of the forces (Section 2.3.2), which minimizes MPI Waitall times.

In the case of a system with 1 billion of particles, we measured a code speed of 0.14 seconds x iteration, which is sufficiently small to enable the study of billion-body structural glasses. Such a system size is two orders of magnitude higher than the largest glass simulation ever reported, and will improve up to two orders of magnitude the resolution of MD measurements on glassy dynamics [13].

4. A glass transition in a 1 billion binary mixture of soft spheres

4.1. A few words about the glass phase

When the temperature of a liquid is reduced below the melting temperature, two possible physical phenomena may occur: either the system undergoes crystallization—a first order phase transition—where the final ordered configuration is the thermodynamically stable phase, or else the liquid may become supercooled and get dynamically arrested into a disordered solid represented by a glass. Despite a large scientific production, the phenomenology of the glass state is still far from being completely understood, and many aspects are yet unknown. As an example, it is not yet clear whether the dynamical arrest is a genuine thermodynamic phase transition, a kinetic phase transition or something else, as the real world counterpart of a phase transition taking place in the trajectories’ phase space as recently suggested by Chandler and co-workers [14].

In the last decades, in particular, several different theories have been suggested and various diverse analysis have been pursued [11, 12, 13, 16, 17, 18]. Notwithstanding the wide diversity of views, a consensus exists over the consideration that a glass transition is a dynamical crossover through which a viscous liquid falls out from equilibrium and becomes solid on the experimental time scale. Such a process is manifested in a gradual change in the slope of the volume (or other extensive thermodynamic variables such as the entropy or the enthalpy) at a specific temperature $T_g$, which defines the glass-transition temperature. A fundamental property of glasses is the existence of a high degree of frustration in their ground state energy configuration [19]. Frustration, in turn, is manifested by the existence a huge number of minima of equivalent energy (metastable states). When the temperature decreases below a specific threshold, the energy barriers of the various minima becomes sufficiently large to trap the dynamics in the configuration space and let it explore only a subset of the available iso-energy surface. The result of this dynamical arrest is a disordered solid that defines the glass phase [18].
Figure 5: Temperature $T$ curve as a function of the time step employed in the study of the liquid-glass transition in a 1 billion particles system.

Figure 6: Caloric curves $U(T)$ obtained from MD simulations (circle markers) and relative least square fit (solid and dashed lines). Figure (b) is an enlarged section of (a) near the glass temperature $T_g$. 
4.2. Sample setup and simulation results

It is worth to mention that on cooling a liquid, if crystallization is avoided, the atomic dynamics is characterized by a relaxation time (naively, one can thing to the typical time needed to change the inherent "configuration") that increase following an Arrhenius law in strong glass forming systems, and even faster in fragile glass forming systems \[20, 21\], reaching the value of 100 s at the glass transition temperature. A supercooled liquid above, but close to, the glass transition temperature can be considered at equilibrium only if its atomic dynamics is investigated for log time, longer that the relaxation time, a macroscopic time. As a consequence, during a MD run, necessarily lasting for time much shorter than the relaxation times close to the glass transition, one falls out of equilibrium as soon as the temperature became that temperature where the relaxation time correspond to the simulation times. As a consequence, in a MD simulation the temperature where the system becomes trapped in a specific inherent structure is largely higher than the real glass transition temperature.

In a molecular dynamics simulation, a liquid-glass transition can be observed as a continuous transition of the extensive thermodynamic parameter as energy or specific volume.

To study this transition, we employed the same binary mixture used for our benchmark suite in Section 3: the high density \( \rho = 1.2 \) and the 20 : 80 highly asymmetric mixture configuration, in fact, neglects the existence of a well defined solid phase for the system and the low temperature ground state becomes highly frustrated \[22\]. We therefore expect the observation of a glass transition in the dynamics as soon as the temperature is decreased to a small enough value. Figure 5 shows the temperature curve employed for our MD simulation. At the beginning, we rapidly increase the system temperature to a high value \( T_0 = 3 \). In this state, the two particles species have sufficient kinetic energy to freely diffuse over the whole simulation box. After 200000 time steps, the temperature starts to decrease by following a slowly-varying linear curve, whose duration is of \( 3 \times 10^6 \) time steps. In order to guarantee stability and energy conservation over the whole simulation, we adopt a time \( t \) resolution of \( \delta t = 10^{-3} \) s. The cutoff range has been set to \( r_c = 1.2 \), which guarantees a sufficiently large interaction distance to observe the formation of a supercooled liquid. Figure 6 displays the caloric curve of the system, and shows the behavior of the potential energy \( U \) versus the temperature \( T \). For temperature values well above \( T_g = 0.2 \), the system is in the liquid state and follows a continuous power law curve with \( T = T_0^{\frac{2}{3}} \), as found from a nonlinear least square fit procedure applied on the energy \( U \) and as expected from the theory of Tarazona \[23\]. As we progressively reduce the temperature beyond the value \( T_g \), we observe the appearance of a continuous transition, characterized by a radically change in the derivative of \( U \) with respect to \( T \). For temperature values below \( T_g \), which defines the glass temperature \[10\], the energy \( U \) varies linearly with the temperature and the system gets trapped into an arrested phase with all the particle oscillating almost harmonically around their equilibrium configuration. Figure 7 displays a 16000 particles portion of the billion-body solid formed at \( T = 10^{-3} \). As expected from the thermodynamic analysis based on the caloric curve, the solid configuration
reached is that of a structural glass, whose particles are randomly arranged in space. The structural properties of the glass are analyzed by calculating the radial distribution function $g(r)$, defined as:

$$g(r) = \frac{2V}{N^2} \left\langle \sum_{i<j} \delta(r - r_{ij}) \right\rangle,$$

(4)

being $V$ the sample volume, $N$ the total number of particles, $r_{ij}$ the distance between particles $i$ and $j$ and $< ... >$ denoting an ensemble average. The radial distribution function describes the spherically averaged local organization around a specific atom, and it measures the probability of finding an atom at a distance $r$ from a given particle. Figure 8 displays the $g(r)$ for the billion-body glass obtained at $T = 0.001$. The glass is characterized by a sharp peak at $r \approx 1$, which yields the average minimum interparticle distance at equilibrium, followed by two broader peaks and a series of oscillations of decreasing amplitude around the asymptotic value $g(r \to \infty) = 1$. The presence of well defined broad peaks in the radial distribution function is the hallmark of a structurally disordered phase, with particles oscillating around randomly arranged spatial sites. This dynamics is smeared out as long as the interparticle distance increases, and all correlations are dramatically reduced after $r \approx 4$, thus indicating the lack of any long range positional order in the system. The $g(r)$ reported in Fig. 8 compares favorably with previous determination in soft sphere systems.
5. Conclusions

We have developed a parallel code which demonstrates the applicability of molecular dynamics techniques to the study of billions-body structural glasses. We tested our code on the world’s largest supercomputer available, namely the Jugene BlueGene system at the Jülich Supercomputing center, and demonstrated scalability on the full machine [characterized by 294912 computing cores] with an efficiency of 89% in the largest configuration of 100 billions of particles. We then applied our code to the case study of the supercooled dynamics of an exceptionally large system, constituted by an highly frustrated binary mixture of one billion of particles. This simulation paves the way to the computational study of billions-body structural glasses, thus achieving new levels of resolution in the analysis of anomalous vibration of amorphous materials and, on broader perspective, of living matter.

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