



# Analyzing molecular dynamics scattered data for large atomic movements



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## ABSTRACT

Molecular dynamics (MD) simulations generally produce massive amounts of data, which contain key structural and dynamical information about the material system under consideration. Information extraction from atomic position-time series is, however, a non-trivial task. It perhaps requires examining the entire data set since it is not known a priori in which parts of the data and in what form the desired information resides. A manual analysis involving all atomic positions at each and every time step is infeasible and ineffective even for moderate-sized data. Here, we develop a system to perform an automatic analysis of MD simulation data sets. Our system focuses on how constituent atoms move and provides an algorithm to automatically identify their movements that are larger than usual oscillating (wiggling) motions in terms of the distance covered within a short time window. The algorithm employs methods from signal processing and uses a regression model to distinguish different types of motions. The system also explores local bonding and structural changes occurring in the time intervals of large displacements, which can perhaps be responsible for structural rearrangement as well as transport phenomena. For illustrations, we analyze the first-principles molecular dynamics simulations of liquid silica ( $\text{SiO}_2$ ) from 2800 to 4000 K at zero pressure. Our system detects, in an automated fashion, numerous significant movements of Si and O atoms, and then associate them to Si–O and O–Si coordination states. The silica liquid is known to form a tetrahedral network mainly consisting of four oxygen coordinated Si atoms and doubly silicon coordinated O atoms (i.e., bridging oxygen). Our analysis suggests that only small fractions of odd coordination states account for the detected large atomic movements. Moreover, threefold coordinated Si atoms and singly coordinated O atoms (non-bridging oxygen) appear to contribute to atomic-diffusion more than pentahedral Si and threefold O states.

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## 1. Introduction

Over the last couple of decades, molecular dynamic (MD) simulation has been one of the most common computational practices in science and engineering. The underlying physical model ranges from relatively simple (empirical) pair-wise interatomic potentials to highly sophisticated quantum mechanical formulation (first-principles) [1–3]. All MD approaches have been adopted in massively parallel environments [4,5]. Pair potentials simulations have been performed for billion atom system and for several nano-seconds [1,6]. On the other hand, first-principles simulations despite being computationally very intensive have also exceeded one nano-second [7] and included several thousands of atoms [8].

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For a given material system, outputs from these simulations represent various physical (bulk) properties including density, compressibility, diffusivity and viscosity [1,2,7,9]. More importantly, they include massive data for atomic configurations, which are distributed in 3D space and vary with time. Gaining insight into useful structural and dynamical information contained in the large-scale simulations has always been highly desirable but still poses a tremendous challenge.

Two types of approaches are commonly used to gain insight into massive data generated by MD simulations. First, numerous visualization systems are currently available to display/render atomic configurations in terms of inter-atomic bonds, modular structures (such as polyhedra, clusters), and other forms [10–13]. Moreover, they support animation and trajectory rendering for a quick navigation through the data. Animation renders the atomic configuration at each time step going through the successive time steps so that one can develop some sense of dynamical behavior.

On the other hand, particle trajectories allow a complete representation of the data by rendering positions of all atoms at all-time steps so full information is contained in a single display [14]. Visualization of trajectories and velocity/displacement data can help us assess the nature and extent of atomic movements. Both the animation and trajectory rendering usually work fine for relatively small-sized data sets. As simulations become larger and longer, frame rates and occlusion become serious issues, and visual inspection becomes less effective. Parallel processing and immersive visualization can be helpful [15,16]. Second, various analysis methods involve computation of system-wide averaged properties [17–19]. They include radial distribution functions, bond length and angle distributions, coordination numbers, ring statistics, etc., to understand structural behavior [12,20]. Similarly, the dynamical analysis involves mean square displacements, bond-event rates, velocity auto-correlation functions, stress auto-correlation functions, etc. Which specific visualization/analysis method works best for a given MD data set depends on the material system simulated and also on its properties being investigated.

In this paper, we propose a useful approach to analyze a given position-time series produced by parallel molecular dynamics simulation for understanding the dynamical behavior of the material system under consideration. In particular, our interest is to explore atomic diffusion, that is, a process by which a material results in the net transport of constituent atoms. While our analysis can be applicable to any type of materials, here we target a liquid (dense) phase. Atomic diffusion in a solid phase is generally too slow to be captured in currently achievable simulation time-scale with any MD approach even at high temperatures close to the melting point. We use silica ( $\text{SiO}_2$ ) liquid as an example in this study [9]. Silica is one of the most abundant materials of our planet and is important from both technological and geological viewpoints. Unlike other liquids, silica liquid is extremely viscous (i.e., highly immobile) so it is interesting to explore how the constituent (Si and O) atoms diffuse or move in this system [1,7]. As shown in Fig. 1, the liquid structure can be viewed as a nearly complete tetrahedral ( $\text{SiO}_2$ ) network. Moreover, it was simulated using first-principles molecular dynamics method, which is generally expected to predict physical (macroscopic-scale) properties with high accuracy so the data may contain meaningful information at the microscopic (atomic) level [9]. In particular, our aim is to identify atomic-level events (i.e., changes in atomic configurations occurring through bond formation and breakage) relevant to a material property such as diffusion. It is likely that such events are confined in both space and time involving few atoms and extending over short time intervals. This implies that only a relatively small fraction of the

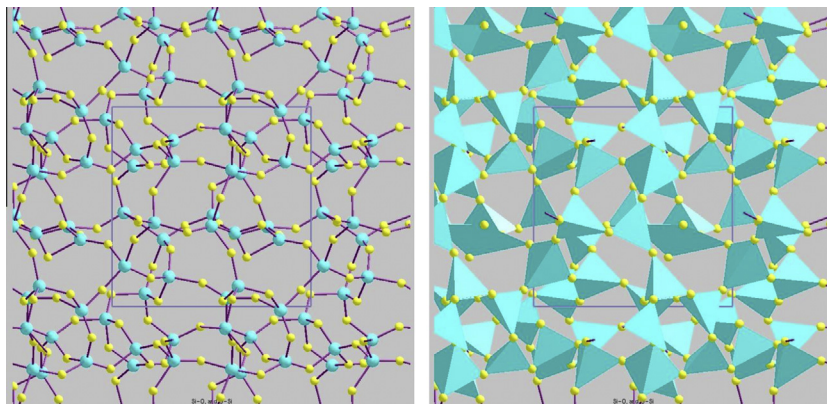
simulation data may actually be worth examining to reveal underlying mechanisms.

The proposed MD simulation data analysis scheme consists of two stages: First, it examines the movement pattern of the constituent atoms, which can involve continuous flowing motion or discrete hopping motion. Using ideas from signal processing, we design an algorithm to automatically detect large jumps in the simulation output that contains both the large jumps and regular oscillations of the atoms. The algorithm also identifies the time intervals in which the large jumps happened if there are any. Second, our scheme describes the liquid system in terms of basic structural units (coordination states representing local atomic connectivity or bonding) and examines how they evolve with time. It relates the detected large jumps to the coordination changes the corresponding atoms undergo. Such coordination change may be part of the atomic level mechanisms that determine the diffusion property of the material. Our results show that the proposed analysis scheme is effective in identifying the large jump moves and the coordination changes that are associated with the movements. It may also help atomistic visualization by pinpointing the time intervals when interesting events likely to occur in the simulation so that we do not need to look through millions of time steps - only corresponding subsets of data may be visualized.

## 2. Material and methods

### 2.1. Simulation data

Data used in this study are from parallel first-principles molecular dynamics (FPMD) simulations of silica liquid [7,9]. The supercell used in the simulations consisted of 72 atoms, which correspond to a discrete set of 216 (positional) degrees of freedom. The atomic positions in liquid phase are strongly correlated but without any long-range order, and are constantly changing with time. The simulation runs ranged from a couple of hundred thousands of FPMD steps (at high temperature of 4000 K) to little more than one million steps (at the lowest temperature of 2800 K studied). A time step of 3 femtoseconds was used at 2800 K so that the simulation duration slightly exceeded 3 ns whereas the time step of 1 femtosecond was used at higher temperatures (3000 K, 3500 and 4000 K). Six data sets (two at 2800 K, two at 3000 K, one at 3500 K and one at 4000 K) were used in our analysis. It is important to note that the simulations are finite in both space and time. The supercell length varies from 10.3 to 13.8 Å whereas the simulation duration ranges from 200 picoseconds to 3.2 ns.



**Fig. 1.** Visualization snapshot of simulated  $\text{SiO}_2$  liquid structure at 3000 K. (Left) coordination view: fourfold coordinated state of Si atoms (cyan large spheres) and twofold coordinated state of O atoms (yellow small spheres). (Right) polyhedral view: tetrahedra formed by Si atoms at the center and four O atoms at the vertices, and bridging oxygens. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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