Molecular Dynamics Simulation and Visualization Parallelism of Structronics

Samira MY Esbitan 1, Thar M. Badri Albarody 1

1 Department of Mechanical Engineering, Universiti Teknologi Petronas, Malaysia

E-mail: samira_g02794@utp.edu.my

Abstract. Computer simulations of Structronics systems require a model reflect thermomechanical reality. A model consists of both a representation of the Structronics system and a set of thermomechanical rules that describe the continuum behavior. However, molecular dynamics is a computer simulation technique able to express the specification and ultimate details of the initial thermomechanical state of Structronics system, and a specification of the external electromagnetic influences at the molecular level. A visualization tool uses to visualize the Structronics molecule motions, interaction and trajectories then to observe the continuum behavior and predict structure performances. Both molecular dynamics model and the visualization tool would be implemented in the framework of parallel computing in order to possess accurate and efficient simulation. Nevertheless, the parallel computing is a group of independent processors working to solve a large computational problem which required a huge effort to utilize larger storage resources and to reduce the execution time. In this paper we propose an approach for developing an integrated molecular dynamic simulation and visualization solution to provide online visualization.

1. Introduction

Structronics are smart (e.g., adaptive, functional or responsive) composite structures that contain the main structure and distributed electronics materials such as: piezomagnetic, piezoelectric, magnetostrictive, electrostrictive, and a like material refer to a class of contemporary structures [1, 15]. They are capable of instantaneously sensing, and consecutively actuating to eliminate the disturbance effects and respond the attractive ones [16].

However, unlike traditional composite, structronics required a special engineering at molecule level to design and disturbed the electronic materials within structure gaining much redundant functionality. On the other hand, structronics adaptiveness, and responsiveness processes cannot be described nor understood in their entirety in a continuum model, but have to be scrutinized with molecular or atomic models [3, 7, 9].

Although the laws of classical mechanics were first postulated to engineering large-scale structures, they turn out to be a surprisingly good approximation at the molecular level where the true behavior is correctly described by the laws of quantum mechanics. Indeed, an entire computational methodology, known as molecular dynamics, is based on the applicability of the laws of classical mechanics to microscopic systems. Molecular dynamics has been remarkably successful in its ability to predict macroscopic thermodynamic and dynamic observables for a wide variety of systems using the rules of classical statistical mechanics [8, 14, 20].
Thus expecting, molecular dynamics simulation would allow us to measure directly the properties of structronics systems which no real experiment could provide such detailed information. Rather, classical experiment measures properties averaged over a large number of distributed electronics systems within the structure and, usually, also averaged over the time of the measurement [13-19].

2. Molecular Dynamics
Molecular dynamics is a form of computer simulation for estimating motions of molecules and strain of atomic bonds. Atoms and molecules are allowed to interact for a period of time by approximations of known physics. By means of prediction of molecule motions, molecular dynamics model able to compute structure strain and stress of solids, as well as shear stress and pressure of liquids, and gasses of material. The main idea is to describe the motion, which how molecule positions, velocities, and orientations, change during the time. It constitutes a motion picture that follows molecules as they move to and fro, twisting, turning, colliding with one another [17-22].

![Figure 1. Typical Molecular Dynamic Simulation Procedure](image)

In the beginning, a sample is assembled based on a model system consisting of N atoms and solved using Newton's equations of motion until the properties of the system reached to the state of equilibrium. Then, actual measurements are applied. The observable quantity is expressed as a function of the positions and momenta of the atoms in the system [1].

The best introduction to typical molecular dynamics simulation procedure is shown in Figure 1.

2.1. The need of Visualization
Molecular dynamics simulations are used to generate trajectories containing atomic coordinates and other dynamic data for individual atoms and molecules. In addition to these properties and behavior we observe, if we can also generate animation of the movement of molecules. Without seeing any real molecules in a system, we can assume that molecules moving in a computer behave much like real molecules. This assumption is supported by the fact that a number of experimentally accessible quantities have been reproduced well by computer simulations.

2.2. The challenges of Molecular Dynamics
The basic problems that are encountered in the computer simulation of molecular dynamics are:

2.2.1. Large data volumes:
The molecular dynamics simulation studies are performed in a time-step from Picoseconds to nanoseconds to milliseconds. Each time step is saved and motion of the molecules changes in each step. As
molecular dynamics need is a time dependent system and each frame of time carries lot of information related to behavior, interaction and properties, analysis and proper understanding is very important. However, just with large data set, one cannot do anything. Hence there is a need for a visualization tool [7].

2.2.2. Three-dimensional configuration of the molecules:
The molecules are oriented in space. Consider each molecule a data point. To know the exact position of each point, one needs X, Y and Z coordinates. And lot of times in experiments, some atoms or catalysis or atom of particular interest is so clustered between the bulk of atoms that the Visualization tool imposes a graphical challenge for the designer or developer. The atoms are so close to each other that physically able to separate them to see them clearly, needs high end graphical interface and challenge on the code [22].

2.2.3. Large number of atoms in each frame:
As trajectories are important for understanding properties of the substance, the results from the simulation studies is temporal. Typically, there are thousands of thousands of atoms in each time step. These atoms are carried to the next time step and hence, understanding of each data point is a serious business. In our typical example we are working on 300,000 atoms with 16 time frames. And this is a huge amount of data to process and prepare for visualization [19].

2.3. Existing Visualization Tools for Molecular Dynamics Simulation
A number of visualization tools have been available on the market in the field of Molecular dynamic simulation visualization tool and to begin introducing a few are:

1. **Visual Molecular Dynamics (VMD)** Visual molecular dynamics (VMD) is a molecular graphics program designed to display and analyze of molecular assemblies, mostly in biopolymers like proteins and nucleic acids. It is written in C++, using an object oriented design. It has a wide variety of rendering styles and coloring methods in order to display any number of structures. It provides a graphical user interface for program control and text interface using Tel embeddable parser. It can also animate molecular dynamics simulation trajectories [19].

2. **gOpenMole** is an open source tool to visualize and analyze of molecular structures and their chemical properties. This program uses Tcl/Tk scripting engine and is extensible to Linux and Windows. It is implemented using SGL OpenGL graphics libraries. Visualization capabilities include displays as a stick, licorice, ball-and-stick, cpk, ball-and-stick with molecule parts colored with selected colors, licorice, and cpk, licorice in stereo. It can also display with rendering different colors for helical protein structure. Atomic density can be displayed in orbit, Connolly surface or cut plane along X, Y and Z axis. Animation also includes travel of molecules in X, Y and Z planes [16].

3. **UCSF Chimera** UCSF Chimera based on Python Programming language. UCSF Chimera is an extensible program for interactive visualization and analysis of molecular structures and related data, including supramolecular assemblies, density maps, docking results, sequence alignments, trajectories, and conformational ensembles. High-quality images and movies can be rendered [17].

2.4. Parallel Computing
Parallel computing is a group of independent processors working to solve a large computational problem which required a huge effort to reduce the execution time and to utilize larger storage resources. Essentially, parallel computing is to partition and distribute the computational work among the involved processors [2, 3, 22].
The Message Passing Interface (MPI)

"Message passing is widely used on certain classes of parallel machines. Designing MPI use of the most attractive features of a number of existing message passing systems, rather than selecting one of them and adopting it as the standard" [2]. Portability and ease-of-use are the key advantages of establishing a message-passing standard. The benefits of standardization are particularly apparent in a distributed memory communication environment in which the higher level routines and/or abstractions are built upon lower level message passing routines. The main goal of the MPI is to develop a widely used standard for writing message-passing programs. As such the interface should establish an efficient, practical, flexible, and portable standard for message passing. The interface should be designed to allow for thread-safety.

3. RELATED WORKS

Molecular simulation is being progressively used to study a widening range of both fluid phenomena and molecular systems. Nowadays, many simulators aim to study complicated molecules such as proteins, whereas the attention was previously confined almost exclusively to simple atoms and molecules. In a similar way, the simulation of equilibrium phase is quite common. The motivation for the increasing use of molecular simulation can be assign to many factors such as improvements in computer hardware, theory, and algorithms. These novel developments have generated enormous growth in the simulation literature [9]. Richard J. Sadus [9] examines some of the important aspects of recent progress in the use of molecular simulation for investigating fluids. It encloses both molecular dynamic and Monte Carlo techniques providing details of theory, algorithms and implementation.

Meha Garg [6] proposed the basis of developing an in-house tool for analysis and display of simulation results based on OpenGL/GLUT and and Microsoft Foundation Classes (MFC) libraries for high end graphic support. The tool uses the results of simulation studies and converts the data in binary format. This feature is provided offline, so the user can keep the data in binary format before playing the tool. In addition, The proposed tool don’t integrate and provide Molecular dynamics graphical interface, where scientists can carry out molecular dynamic simulation and the results produces from the studies can be used for graphical display [6].

Xue Kong [13] proposed a framework to visualize the abnormal clusters shifting atom groups in a three-dimensional space, and show their temporal relationships. The framework provides a pattern mining method to detect abnormal atom groups which have large variance compared to the majority atoms and share similar movement. Xue Kong provided [13] a general molecular dynamics simulation tool, which can visualize a large number of atoms, including their movement and temporal relationships. Using this tool, it could help domain experts study molecular dynamics simulation results. The proposed framework didn’t provide integrated solution for MD simulation & visualization, thus it still provides offline visualization by using a tool uses the results of simulation studies and converts the data in binary format [13].

4. THE PROPOSED FRAMEWORK

Figure 2 shows the proposed framework to to develop an integrated molecular dynamic simulation and visualization solution to provide online visualization of strucronics.

Procedure of MD Part 1 & 2:

As it shows below in figure 3, the basic MD algorithm will do the following:

1. Calculate how a system of particles evolves in time
2. Consider a set of atoms with positions /velocities and the potential energy function of the system
3. Predict the next positions of particles over some short time interval by solving Newtonian mechanics
Figure 2. Methodology

Figure 3. Basic MD Algorithm

Figure 4 shows how to apply parallelism for MD.

Figure 4. The proposed MD Simulation
Part 3: Parallelize Visualization
The simulation results will visualize by rendering images and animations of the position of the atoms during the time. There is a need to visualize the simulation data by developing a custom program to extract the energy value and the 3D position of each atom. To represent each atom on a produced image, a sphere was generated in Visualization ToolKit (VTK) using the 3D position as the center point of the sphere. VTK primitive tubes will use to create the appearance of a mesh by connecting the atoms’ bonds using a version of the k-nearest neighbor algorithm. The desired range of atoms will be connected with a tube using VTK. Colors will be applied to the spheres and tubes based on the stress and energy values. The ends of the tubes will be colored by the same as the atoms they were connecting, which, in some cases, will require two differently colored atoms. VTK automatically colored the rest of the tube by smoothly blending from one end to another. Figure 5 shows the proposed visualization procedure.

Figure 5. The proposed MD visualization

5. Expected Result
The results can be interpreted with the help of appropriate visualization techniques. Whenever corresponding results of physical experiments are accessible, then the results of the computer simulation can be compared. This leads to a verification of the results of the computer simulation or to an improvement in the applied methods or the model (for instance by appropriate changes of parameters of the model or by changing the used equations).

6. Conclusion
In this paper we propose an approach to developing an integrated molecular dynamic simulation and visualization solution for Structronics. Both molecular dynamics model and the visualization tool would be implemented in the framework of parallel computing in order to possess accurate and efficient simulation.
ACKNOWLEDGMENTS
Authors would like to thank mechanical engineering department, Universiti Technologi PETRONAS for its esteemed support.

7. References
[1] Cai, E. Acklam, H. P. Langtangen, and A. Tveito, 2007, Parallel Computing, Simula Research Laboratory, Oslo.
[2] Blaise Barney, 2014, Introduction to Parallel Computing, Lawrence Livermore National Laboratory.
[3] Włodzimierz Bielecki, Dariusz Burak, December 16-18, 2005, Parallelization of the AES Algorithm, Proceedings of the 4th WSEAS Int. Conf. on Information Security, Communications and Computers, Tenerife, Spain.
[4] J. M. Haile, 1997, Molecular Dynamics Simulation: Elementary Methods, Wiley, John & Sons.
[5] Dennis Rapaport, 2004, the Art of Molecular Dynamics Simulation, Cambridge University Press.
[6] Meha Garg, 2010, Visualization Tool for Molecular Dynamics Simulation.
[7] Markus Buehler, Spring 2008, Introduction to Modeling and Simulation, MIT Open Courseware http://ocw.mit.edu 3.021J / 1.021J / 10.333J / 18.361J / 22.00J.
[8] Hans-Dieter Hölzle, 2003, Wolfgang Sippl, Didier Rognan, Gerd Folkers, Molecular Modeling: Basic principles and Applications, Wiley-VCH.
[9] Richard J. Sadus, 2002, Molecular Simulation of Fluids.
[10] Erik Lindahl, Berk Hess, David van der Spoel, GROMACS 3.0: A package for molecular simulation and trajectory analysis
[11] Michael P. Allen, 2004, Introduction to Molecular Dynamics Simulation, published in John von Neumann Institute for Computing, Jiilich, NIC Series.
[12] Christopher Lewis, Charles Cornwell, July 2016, Visualizations of Molecular Dynamics Simulations of High-Performance Polycrystalline Structural Ceramics, Data Analysis and Assessment Center (DAAC).
[13] Xue Kong, 2014, Pattern Mining and Visualization For Molecular Dynamics Simulation.
[14] William Humphrey, Andrew Dalke, Klaus Schulten, 1996, VMD: Visual Molecular Dynamics, Journal of Molecular Graphics 14:33-38, Elsevier Science.
[15] Samish Milan, May 2005, Protein Motion: Molecular Dynamics, Structural Bioinformatics Course.
[16] Snow CD, Nguyen H, Pande VS, Gruebele M., Nov 7 2002, Absolute comparison of simulated and experimental protein-folding dynamics. Nature 420(6911):33-4.
[17] Stephen Wells, Scott Menor, Brandon Hesperheide, and MF Thorpe., 2005, Constrained geometric simulation of diffusive motion in proteins. Physical Biology 2:S127-S136.
[18] Hans-Dieter Holtje, Wolfgang Sippl, Didier Rognan, Gerd Folkers, 2003, Molecular Modeling: Basic principles and Applications, Wiley-VCH.
[19] William Humphrey, Andrew Dalke, Klaus Schulten, 1996, VMD: Visual Molecular Dynamics, Journal of Molecular Graphics 14:33-38, Elsevier Science.
[20] Toktam Taghavi, Mark Thompson, Andy D. Pimentel, 2009, Visualization of Computer Architecture Simulation Data for System - Level Design Space Exploration. Proceeding SAMOS '09 Proceedings of the 9th International Workshop on Embedded Computer Systems: Architectures, Modeling, and Simulation, Pages 149 – 160.
[21] Samish Milan, May 2005, Protein Motion: Molecular Dynamics, Structural Bioinformatics Course.
[22] H.M. Aktulga, J.C. Fogarty, S.A. Pandit, A.Y. Grama, April–May 2012, Parallel reactive molecular dynamics: Numerical methods and algorithmic techniques, Volume 38, Issues 4–5, Pages 245–259