Virtual Reality Biological Simulation for SMMS Telemanipulation
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Abstract—This paper introduces a molecular mechanics study by using an intermolecular dynamics software (IMD) coupled with virtual reality (VR) techniques, which permits manipulation of molecules in molecular dynamics simulation and 3D graphical display. The main novelty of the proposed simulations is based on the micromechanical and microelastic property characterization of living cells by applying Bilateral SMMS (Single Master Multiple Slave) teleoperation system to manipulate a living cell in their virtual native environment.

Keywords—Virtual Reality, Molecular dynamics, Micro/Nano-manipulation, Haptic, SMMS

1. INTRODUCTION

Recently, the researcher in a field of the biological cell manipulation pays a great effort focused on cell analysis, diagnosis, and manipulation of a living cell which has been gaining prominence in a wide range of applications including, cell stretching, bending, injection, cellular diagnostics, gene and molecular delivery, and single cell-based assays [1]. A living cell manipulation offers much more accurate selection and understanding of cell properties than data-averaging over a population of cells [2]. A manipulation of a living cell is a challenging operation task since it needs not only a precise, controllable manipulator set-up but also a suitable end-effector which can be actuated to accurately perform specified tasks without the excess of the force which damages the cells. Therefore it is preferable to understand the interaction, characteristic and properties of a desired sample before performing the real operation.

In this work, we consider a molecular mechanics study to improve the methodology of mechanical molecular studies of grasping and moving a Deca-alanine [3] which is a peptide composed of ten alanine residues and considered as a target object. In order to investigate the behavior and properties of a Deca-alanine such as micromechanical and microelastic properties, we simulate two micro/nano manipulator’s tips (slave) to grasp and move a virtual Deca-alanine. The interaction force of the micro/nano manipulator’s tips and Deca-alanine during the operation is calculated based on the IMD software and 3D visual display is shown by VMD (Virtual Molecular Dynamics) software [4]. By performing the simulation of a Deca-alanine manipulation, we can not only predict the type of force spectra and irreversible work that may be occurred from a Deca-alanine manipulation experiments, but the molecular mechanic behavior, control Deca-alanine’s parameters could also be more understood, which will be useful for performing the real operation and performance evaluation.

2. MOLECULAR DYNAMIC SIMULATION AND VIRTUAL REALITY

To achieve the above long-term goals, interaction molecular dynamic (IME) simulator is one of necessary tools in order to understand the molecular mechanics of living cells or any biological object, develop dynamic, kinematic models, and study their performances and control aspects. Moreover, the IME simulator could be used together with the VMD simulator to provide us an ability to visualize the atom-atom interaction and display the results in fully immersive 3D environment in real-time.

The overall proposed system is presented in Fig. 1 which permits a manipulation of bio-nanorobotic components in MD simulations, 3D graphical display in real-time. The system mainly consists of three main components: 1) a mouse or a PHANTOM haptic device (future work) which permits an operator to apply a environment or external force to virtual model in the system as well as feel the force feedback during the operation, 2) a NAMD (Numerical Analysis Molecular Dynamics) [5] simulation which is used to assess the influence of Ph value, temperature change, electron density or salt concentration, calculate the effect of the force and analysis the atom-atom interaction under external constraints, 3) a VMD (visual molecular dynamics) software which is used to visualizes a complex architecture and interactions of bio-nanorobotic and display the results.
in 3D graphic in real-time.

Each component of the system are connected by an efficient protocol such as TCP/IP to achieve the communication between the VMD, NAMD running on a single computer or extended to multiple computers for a huge mass calculation data. An operator can exert a force, external constraints to the system through the using of a simple mouse or a PHANTOM haptic device (future work) which measures an operator hand’s position and exert the force according to the movement of an operator hand’s position, thus an operator is able to apply different mechanical constraints, external force, and energy fields to the virtual model in the system depending on the desired task operations.

3. SIMULATION RESULT

Fig. 2 The 3D graphic of Deca-alanine in an alpha-helix structure form with six Hydrogen bonds (white dash lines) (a) and with three hydrogen bonds left (b)

(a) An initial state

(b) A final state

In this section, the proposed system is used to perform a simulation of a manipulation of Deca-alanine. In this simulation, we simulate a Deca-alanine in vacuum under the CHARMM force field environment [6] and a temperature of 300K is constantly maintained as well as van der Waals interaction and electrostatic interaction occurs between each atom and bond are also taken into account in this simulation. Deca-alanine forms an alpha-helix in vacuum environment because the alpha-helix is the stable conformation of the molecule in vacuum. Fig. 2 shows Deca-alanine in an alpha-helix structure in vacuum. It is composed of ten alanine residues and is stabilized by six hydrogen bonds and its length is about 12 Å. The task shown in Fig. 3 is to grasp an object (Deca-alanine) at the start position by applying force at a head and a tail of Deca-alanine atoms shown by 2 red atoms, then lifting, moving, lowering, and finally releasing it at the target position in 70 ps. A constant force is applied to 2 atoms by 7.2 kcal/mol/Å² from 0 to 70 ps. In Fig. 4, the trajectory of two atoms (red) which are pulled by applying external force in the pick and place simulation. We can observe that at initial position 0 ps, there are six hydrogen bonds which stabilize Deca-alanine’s alpha-helix structure but after being pulled at both head and tail parts of Deca-alanine atoms, we can see that three hydrogen bonds are broken due to the pulling force occur in the simulation. Also a distance between two atoms (orange) that holding a hydrogen bond versus a time is shown in Fig. 5, we can observe that one of six hydrogen bonds is broken at a time about 28 ps (red circle mark).

Fig. 3 The 3D graphic of Deca-alanine during Pick and Place task taken in 70 ps, (a) initial state (b) lifting state (c) right movement state (d) after lowering, final state

Fig. 4 The trajectory of two atoms (red) that are being pulled by applying external force during the pick and place task in 70ps, (a) initial state (b) lifting state (c) right movement state (d) final state
4. CONCLUSION

In this paper, we propose a molecular mechanics study by using an intermolecular dynamics software (IMD) coupled with real-time fully immersive virtual reality simulation for a biological SMMS manipulation system. The position, force, energy feedback are measured and analyzed for the micromechanical and microelastic properties of living cells such as a Deca-alanine. These data are needed and useful for the actual operation. In the future work, we will integrate a PHANTOM haptic device into a proposed system which allows the operator to exert the force, external constraints on the virtual sample as well as feel the force feedback during the operation in real-time. The bilateral SMMS teleoperation system configuration [7,8] is used to control the PHANTOM haptic device(master) and two virtual manipulators for the pick and place task. With a PHANTOM haptic device integrated system, operator could not only manipulate or exert an external constraints on the virtual sample but operator could also feel a very small scale of force feedback in nano scale during the simulation in real-time, which will give a higher accuracy and more reliable biological manipulation operation with higher successful rate in various tasks such as stretching, bending, injection, and pick and place tasks.

REFERENCES