Restraint-based 3D Shape Manipulation Method using Hand Gestures for Interactive Molecular Dynamics

Ryohei Suzuki, Daisuke Komura, Shumpei Ishikawa

Department of Genomic Pathology, Medical Research Institute, Tokyo Medical and Dental University, 1-5-45 Yushima, Bunkyo-ku, Tokyo, 113-8510 Japan,

{rsuz.gpat, dkom.gpat, sish.gpat}@mri.tmd.ac.jp

Kazuki Yamamoto

Laboratory for Systems Biology and Medicine, Research Center for Advanced Science and Technology, The University of Tokyo, 4-6-1, Komaba, Meguro-ku, Tokyo 153-8904, Japan,

kayamamoto-tky@umin.net

Steered Molecular Dynamics (SMD) is widely used for hypothesis verification about behaviors of molecules, especially proteins and ligands, by applying external forces to atoms in simulated systems. [1, 2] Interactive Molecular Dynamics (IMD) provides its user with a real-time visualization of SMD calculation and control of external forces given to atoms to make full use of biological knowledge and human's empirical insight in simulations and to improve understandings of molecular behaviors. [3] Enabling the users to cultivate their insights of molecular behaviors from interactive experience in simulated systems and reflect them back to it is the most important contribution of IMD. [4] Thus the input method for specifying external forces given to atoms is a central problem of IMD system design.

The current mainstream input method used in IMD systems, which probably owes its basic idea to that of SMD, is explicit specification of external forces on each atoms or atom groups by pulling them to target directions on display using variety of devices including mouse, haptic devices and smartphones. [5] While some input methods with 3D tracking devices are proposed to enable users to use their gestures for operation, most of them also consider only single or several points in space represented by user for specification. [6]

When we humans manipulate a shape of something in real world such as clay, we do not usually pay attentions in certain points of an object to make it arbitrary shape, but we impose a global restraint for the shape, like a mold, by pressing the object with our palms, fingers or some surfaces. In such situation the external forces given at each points of the object are

decided implicitly and dynamically by the restraint. We think the lack of such implicit and dynamic property of input method in current IMD systems makes it difficult to manipulate molecular structures using intuitive actions like twisting, stretching or bending.

We propose a new input method for IMD system which uses 3D tracking devices to capture hand gestures of a user to specify constraints of molecular shape, not a force directly, to realize an intuitive interaction style for IMD, where a user can manipulate molecules as if he/she is really touching them. In our method the hands of a user are captured by 3D tracking device and a pair of virtual hands are generated in simulated system. By pushing the virtual hands to a molecule, forces are applied to atoms that touch them. Because contact between atoms and the virtual hands are always taken place through movement of the hands or transformation of the molecule, the distribution of forces given to atoms would be changed dynamically during a simulation. Using our method complex manipulation of molecular structures in IMD may become able to be done relatively easily. We will show examples of applying our method for understanding of some protein-protein or protein-ligand interactions.

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