# MOLding: Gesture-based Interactive Molecular Dynamics for Protein Structure Manipulation

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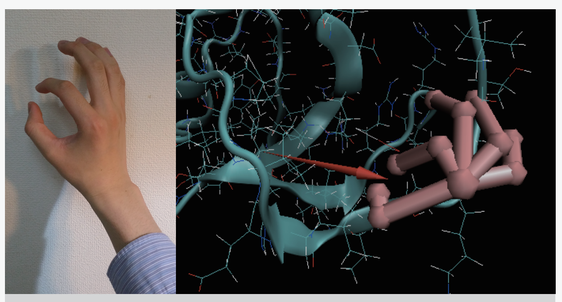
## Introduction

Molecular Dynamics (MD) provides various insights for understanding biochemical reactions. Interactive Molecular Dynamics (IMD) is a derivative technique of MD that permits manipulating molecules in MD simulations by allowing users to apply external forces to atoms in a simulated system, and widely used in biochemical researches. However existing IMD systems [1,2,3] provide several interfaces for specifying given forces for atoms, it is still difficult to manipulate larger structures of molecules in IMD systems. We implemented a novel input method for IMD that enables users to use their hand gestures for manipulating larger molecular structures, by extending VMD[4]. It measures user's hand gestures with Leap Motion device, and generates a set of virtual hand models in the simulated system that behaves in synchronization with the real hand. User can apply external force to atoms by touching them by the virtual hands in multiple modes associated with different gestures to manipulate molecules in effective ways.

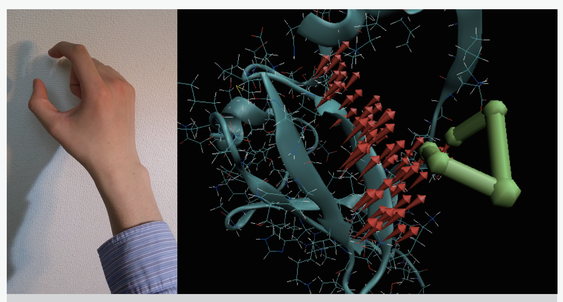
## Gesture-based Interactions

Reflecting our intuition in real object manipulation, we defined five gestures for interacting with molecular dynamics simulation with distinct functions for each.



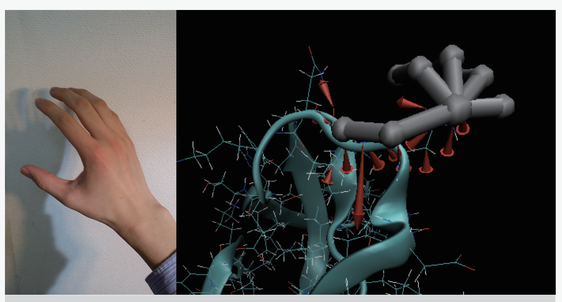
**Pinching**

User can pinch an atom by their index finger and thumb, and apply force to it toward the position of the tips. The magnitude of the force is determined in linear to the pulling distance, like a Hooke's spring.



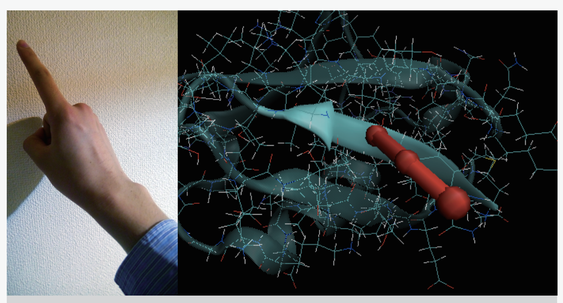
**Holding**

User can hold a secondary structure of a protein by their hand, and apply external forces simulaneously to the all atoms in it to manipulate it in 6-DOF manner, by moving and rotating the holding hand.



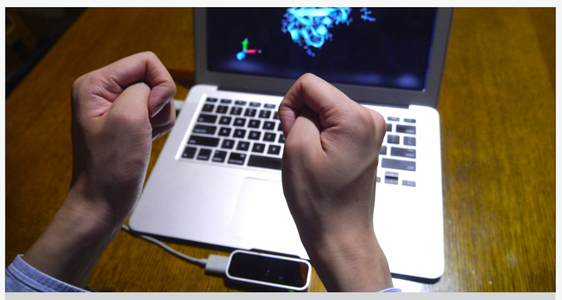
**Pushing**

User can open their hand to enable pushing mode. In this mode, user does not set applied force explicitly, but specifies constraints that give repulsion force to contacting atoms by their hand shapes.



**Pointing**

Pointing gesture is used to mark a certain region of a molecule to be manipulated by pinching, holding and pushing modes. After pointing, only the marked region become the subject of external force.



**Steering**

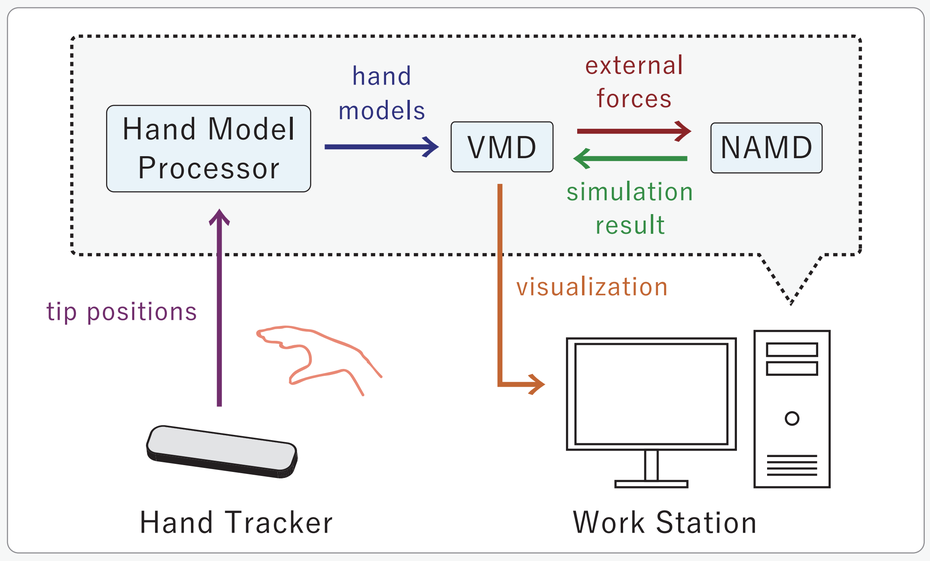
User can navigate the scene view with their grasping hands. The correspondence between their movements and the navigation is defined like transformation of a rigid body holded by two hands.

Usage image

## System Implementation

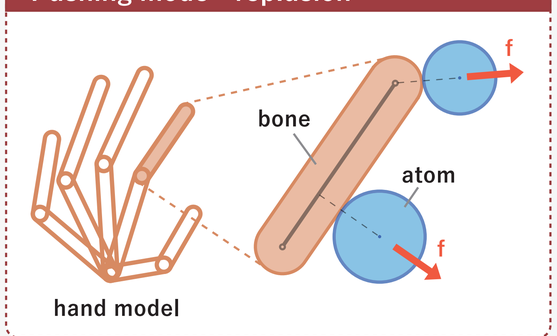
MOLding is composed of a MD simulator (NAMD[5] or GROMACS), modified VMD software and a hand model processor. We used the existing IMD framework implemented on NAMD and VMD for providing the basic IMD functions, and added the gesture-based interaction feature to it. The hand model processor constructs hand models from raw data measured by Leap Motion device, and sends it to VMD.

**System overview**

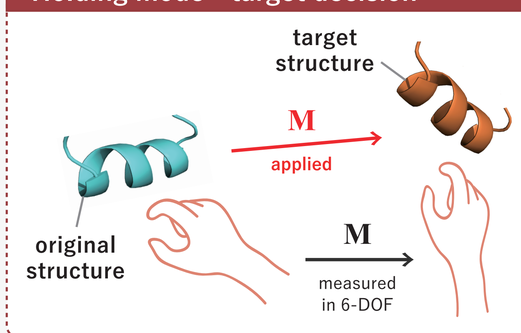



In pushing mode, an atom contacting the hand model is given external force with the direction perpendicular to the surface of the contacting position of the bone. In the other modes, hand movement is measured in 3-DOF (pinching) or 6-DOF (holding). Then it is applied to captured atom positions to obtain the target positions.

**Pushing mode - replusion**




**Holding mode - target decision**




## Conclusions

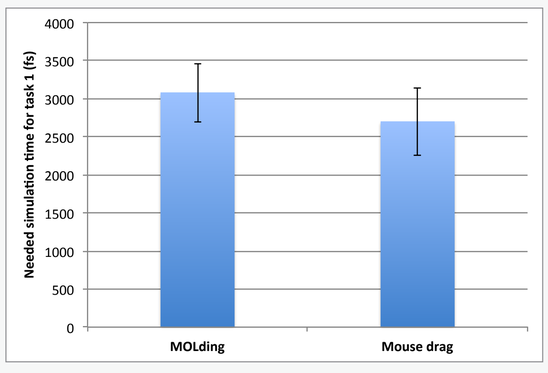
We developed MOLding, a novel input method for interactive molecular dynamics, in which user can control the external forces using their hand gestures in intuitive and efficient ways. The evaluation results suggested that the users were able to perform a simulation task using MOLding in comparable time with conventional mouse dragging method, and in some cases, our method gives better performance.

As the future work, we will continue to improve the input method for providing more intuitive experience, such as adding visual feedback to user input based on simulated molecular behavior. Also, we will conduct more detailed performance evaluations on the system to verify the usefulness of MOLding in actual researches.

## Evaluations

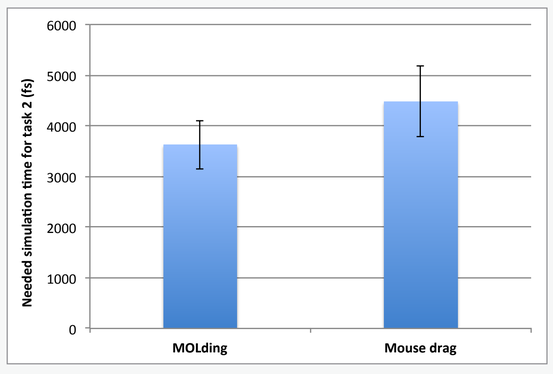
We conducted a performance evaluation consisting of two user tests. Each test requires a participant to complete a protein manipulation task in an interactive MD simulation using either conventional mouse dragging or our MOLding system.

**Task 1: protein unfolding**




In task 1, participants unfolded the structure of a single chain ubiquitin molecule made up of 76 amino acids (1UBQ) by IMD, and the needed time steps to dissociate the all intramolecular hydrogen bonds except for intra-helix ones was measured.

**Task 2: protein-ligand manipulation**




In task 2, we used a protein-ligand system (1VGH) where HIV-1 protease homodimer is complexed with a small molecule. The task was taking the ligand from the pocket on the protein homodimer, and put it back to the pocket from the other side.

## References

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