Visual and Force Feedback-enabled Biomolecular Docking

The computer graphics methods and techniques allow real-time interactive visualization and manipulation of 3-dimensional (3D) objects in virtual environment. The assembly of molecules in a 3D space or molecular docking is used for rational drug design. These techniques help the user to understand molecular interactions and to evaluate the design of pharmaceutical drugs. In recent years, besides the visualization techniques, there has been increasing interest in using haptic interfaces to facilitate the exploration and analysis of molecular docking. Haptic device could enable the users to manipulate the molecules and feel its interaction during the docking process in virtual laboratory or even in shared collaborative environment. Research group led by Asst Prof Olga Sourina is working on methods and algorithms for haptic-based docking in a Virtual Reality (VR) environment to predict favourable transmembrane helix interaction. The project has two main directions. First, we develop molecular docking system that can be used both in research and education. The system is implemented as a stand alone application, and currently we are working on its implementation in collaborative virtual environment for educational application. Second, we develop helix-helix docking system that is a part of biological research conducted in SBS. Currently, we are developing a prototype of Transmembrane α-helices Docking System HMolDock (Haptic-based Molecular Docking) using the haptic device PHANTOM 1.5/6DOF (6 degrees of freedom). The project is supported by 3 years MOE research grant RG10/06. This is an interdisciplinary research in collaboration with School of Biological Science.

The visualization and haptic rendering methods and algorithms developed in this project are applied in other research projects such as Virtual Orthopedic Surgery, Visual Data Mining, etc.

Interaction of αIIb integrin transmembrane helix and a designed antibody-like complementary peptide anti-αIIb.

The students developing visual haptic-based molecular docking system.