University of East Anglia

SYS CONSULTING

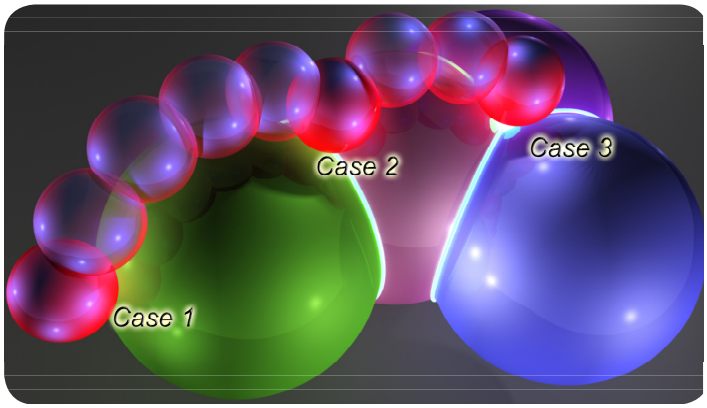
Haptics

# Touching Proteins: A Pioneering Haptic Rendering Algorithm for Molecular Interaction

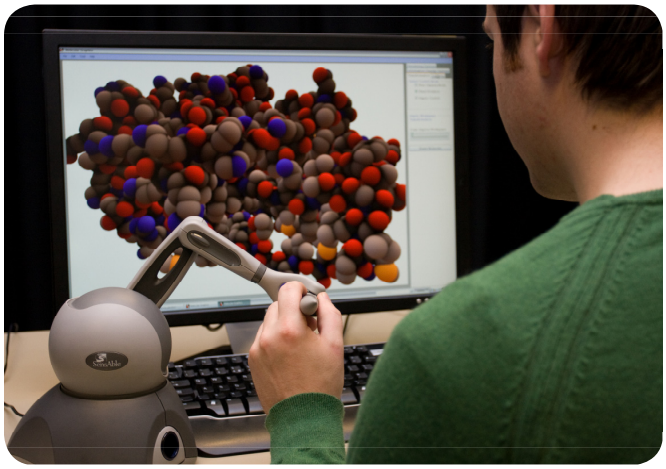
## Business Challenge

The sense of touch can be used to augment our visual sense to gain a deeper insight into the three dimensional shapes of complex objects. Biomolecules are examples of highly complex three dimensional objects which are often visualised using molecular graphics. The augmentation of our sense of sight with touch would be a useful aid in understanding the overall three dimensional shape of a biomolecule. In addition if our probe for touching the protein surface were the size of a water molecule one could also determine solvent-accessible regions of the biomolecule.

Modelling touch requires a force feedback or haptic device capable of exerting forces on the user. These forces are computed based on the position and orientation of the end-effector of the haptic device at a rate of 1000Hz, to ensure smooth and stable forces are perceived. The process of determining the forces transmitted to the haptic device is known as haptic rendering and in this case works by computing forces of interaction between the three-dimensional cursor and the simulated biomolecule.




*Above: A trace through all three states of the algorithm. As the user manipulates the haptic device the smaller sphere will move, constrained to the surfaces of the overlapping spheres forming the molecule.*



*Above: User manipulating the haptic device to interact with the molecule (liver dehydrogenase, LADH) visualised on the monitor.*

## Our Solution & Expertise

Our approach is quite different to previous applications of haptic rendering in the area of biomolecular simulation.

Our application enables the user to employ their sense of touch in order to gain an insight into the three-dimensional shape of a complex biomolecule and, by using a “cursor” that is the same size as a water molecule, hard-sphere interactions with the biomolecule can be calculated to determine regions on the molecular surface that are accessible to water.

## Business Benefits

Researchers working in the School of Biology have utilised the system to investigate new channels in their proteins, that previously had gone unnoticed. Future research aims to incorporate the dynamic properties of proteins during the molecular interactions.