

Poster I-81

Improvement of Portable virtual reality system with haptic device for molecular modeling and education.



Authors:

Isao Okada (*Tokyo Medical and Dental University*)
Takayuki Ohnishi, (*Tokyo Medical and Dental University*)
Hiroshi Nagata, (*Tokyo Medical and Dental University*)
Hiroshi Tanaka (*Tokyo Medical and Dental University*)
Hiroshi Mizushima (*Tokyo Medical and Dental University*)

Short Abstract: We have been developing Virtual Reality System for molecular modeling using haptic device. This time we have improved our easy-to-carry system for demonstration at the conference or at other labs using portable PC. We also tried some actual simulation of membrane proteins.

Long Abstract:

Introduction.

Computational drug design has been mainly done by calculation of the molecular dynamic energy and seeing its structure on CRT. We had to make the 3D structure in our mind by display with rotation or 3D view. Also, molecular binding simulation of two molecules is calculated by the force between the molecule and the protein was just minimized or simulated dynamically. To realize this kind of process, so that human experience can help the drug design, we have been trying to develop a system so that we can touch and feel the protein and the interaction of a compound to it.

We have developed a system using haptic device to perform this simulation, however, calculation need large server for real-time energy calculation, and it can be done only at the place where we place our calculation parallel servers.

This time, we have improved the system with small PCs so that we can carry out for demonstration. Evaluation of this system is only possible by touching it, so this was important to let many people use the system. We also tried some molecular simulation of membrane proteins.

This system is applicable not only for drug design but also for teaching chemical reaction and/or molecular docking etc.

System,

Three portable PC (Pentium M, 755, 512M memory) has been configured to do the parallel processing of the energy potential and controlling haptic device. Graphics are handled on the other PC operating on Linux with naked eye 3D display (Sharp Mebius). 3D technology was enhanced by Interactive Stereo Library for Linux by SGI.

Results and Discussion

The performance of the system is slower than the bigger configuration, but it is acceptable for first time demonstration. It is also acceptable for educational use for touching low molecular weight compounds. .

It is still too large for shipping for demonstration to the conference oversea (like this time to ISMB), however, it is now possible to send to domestic conference as the system is much smaller than it was before.

We also tried some molecular simulation of membrane proteins. Membrane proteins are stabilized in the lipid bilayer and hard to simulate, so we had to perform some approximation. We are now trying to enhance our high performance molecular VR system by enabling to change the local structure of the protein. This requires another big capacity of calculation time, and seems not possible with a small system. We will continue to develop both high end system and easy configuration system for both research and education.

Acknowledgement

This work has been supported by Grants in aid from Ministry of Education Culture Sports Science and Technology of Japan. We thank Mr M.Hatsuta and Mr. D.Arai of Mitsubishi Space Software Co. for coding the software.

References

Mizushima H., Nagata H., Tanaka E., Hatsuta M., Tanaka H.; Virtual Reality System using Force Feedback Device for Molecular Modeling. MEDINFO2001 (V.Patel et al. Eds. Amsterdam:IOS Press pp.975-978 (2001)

Nagata H., Mizushima H., Tanaka H.; Concept and prototype of protein-ligand docking simulator with force feedback technology. Bioinformatics Vol.18 No.1 p.140-146 (2002)

Mizushima H., Tanaka H., Hatsuta M., Arai D., Nagata H.; Molecular Modeling using Virtual Reality with Force Feed Back. 11th International Conference on Intelligent Systems for Molecular Biology (ISMB) (2003)

Isao Okada, Takayuki Ohnishi , Hiroshi Nagata, Hiroshi Tanaka, Hiroshi Mizushima ; Portable virtual reality system using haptic device and naked eye 3D display, for molecular modeling. 13th International Conference on Intelligent Systems for Molecular Biology (ISMB) (2005)