4-1-2012

A Three-Dimensional Visualization and Projection Workbench for the Pace HPC Initiative

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Progress Report: ThinkFinity Grant

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May 29, 2012

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Purpose

The purpose of this project is to build a visualization workbench that supports the Pace High Performance Computing (HPC) Initiative in several ways:

A. Visualization

1. Allow design and building of molecular models and systems using force-feedback and 3D stereographics that will be submitted to the HPC cluster for further computation and refinement.
2. Allow real-time interactive force-feedback sensing and 3D stereographic visual analysis of molecular systems computed on the HPC cluster that includes the output of quantum mechanical, molecular mechanical and molecular dynamic simulations.
3. Provide an experimental test bed for investigating real-time molecular docking and interactive molecular dynamics of prototype systems.
4. Supports classroom demonstrations of above.

B. Projection

1. Develop a portable system for 3-D stereographic projection for seminar projection
2. Develop a local system for interactive 3-D stereographics in intimate setting.

Progress to Date

Parts of the prototype system were ordered in January and February 2012. By mid-March all essential components for a basic test system had arrived and initial assembly began. The prototype system is comprised of a: INTEL XEON W3565 processor, with 8 GB RAM, 500 GB Hard Drive, 2GB Nvidia Quadro 4000 stereographic video card, Acer HN274H 27" Stereo 3D LCD Display, Windows 7 64 bit OS, and a Sensable Phantom Omni 6DOF haptic interface. System software was upgraded and drivers for all special hardware were installed.

Molecular visualization software was installed on the computer system, including the programs: VMD [1], PyMOL [2], Swiss PDB Viewer (DeepView) [3], UCSF Chimera [4], and Accelrys DS Visualizer [5]. All these programs were tested with the basic 3D stereographic display hardware. In addition, the HaptiMOL program by Stocks, Laycock, and Hayward was installed and tested [6]. HaptiMOL uses the Omni Phantom haptic device to allow a user to feel a molecule's solvent accessible surface, and apply forces to a molecular model and view its resulting deformation.

Work began on building software so the system could be used for interactive molecular dynamics (IMD) and steered molecular dynamics (SMD) [7]. This system requires three components: the NAMD molecular dynamics package [8], VMD, and VRPN, the Virtual Reality Peripheral Network [9], which provides a haptic interface to the Omni Phantom. Currently, the VRPN server is being built to interface with both the VMD molecular visualization software and the NAMD molecular dynamics package.

Future Work

Summer 2012 will be used to complete the construction of the force feedback system and test real-time docking. During Fall 2012 the system will be expanded to meet the requirements for 3D projection and demonstration.

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