INTRODUCTION

A modular architecture for high performance applications

The FvNano platform is based upon FlowVR, a middleware made to ease the development of interactive software on HPC platforms. FlowVR itself is a suite of libraries that will handle display, interaction peripherals and data exchange. The figure on the left illustrates the different data flows used in the FvNano project.

The use of this particular kind of architecture has been motivated by the possibility to easily add new functions by integrating new modules. Hence, the user does not have to modify the existing source code and it allows him to share his newly created modules with the community.

As a FlowVR application, FvNano can be launched on computer clusters with little configuration. No change of code is necessary as FlowVR handles all data exchanges between the nodes natively on these environments.

APPLICATIONS AND PERFORMANCE

Interactive Molecular Dynamics

With the interactive dynamics application, the user can manipulate the atoms of a molecular structure and feel the force he is applying to it with the Phantom haptic arm. As a molecular dynamics engine is running in the background, the user can choose which atomic forces will be applied to its system.

As of now, the supported interaction peripherals are the mouse, the SpaceNavigator (3D mouse) and the Phantom haptic arm.

The IMD application has been launched on a 15 nodes cluster with an increasing number of CPU cores using a 170K and 305K atoms systems. Results are shown on the right. Further tests are in progress, with bigger molecular systems and using more CPU cores.

Trajectory Reader

Molecular simulations are difficult to visualize as one often has to extract “still” pictures out of them because of the large quantity of data to handle. Similar to a video player, the Trajectory Reader can load a molecular trajectory computed by GROMACS and display it with the same controls (play/pause/rewind, etc...). The application works for a wide variety of molecular systems.

The figure above shows the performance gain of the application when the number of CPU cores is increased.

Screenshot of the Trajectory Reader application, various analysis tools will soon be added.