FvNano

An Interactive Molecular Dynamics platform

http://www.baaden.ibpc.fr/projects/fvnano

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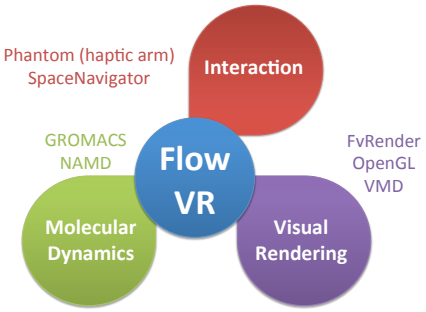
INTRODUCTION

A modular architecture for high performance applications

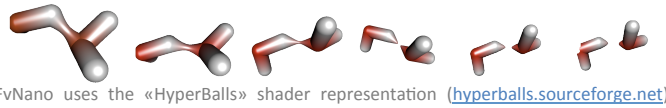


The **FvNano** platform is based upon **FlowVR**, a middleware made to ease the development of interactive software on HPC platforms. FlowVR itself is a suite of libraries that will handle display, interaction peripherals and data exchange. The figure on the left illustrates the different data flows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

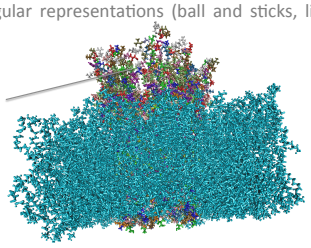
The use of this particular kind of architecture has been motivated by the possibility to **easily add new functions by integrating new modules**. Hence, the user does not have to modify the existing source code and it allows him to share his newly created modules with the community.

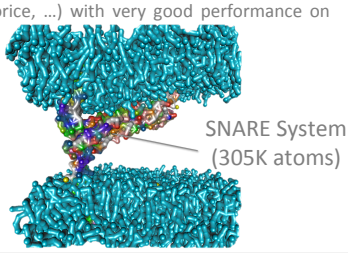
As a FlowVR application, **FvNano can be launched on computer clusters with little configuration**. No change of code is necessary as FlowVR handles all data exchanges between the nodes natively on these environments.

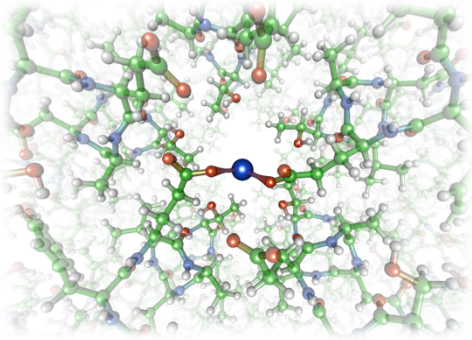
To visualize and manipulate complex molecular systems



FvNano uses the «HyperBalls» shader representation (hyperballs.sourceforge.net) which helps visualize non covalent bonds, as shown above with a two water molecules dynamic. The shader can also render regular representations (ball and sticks, licorice, ...) with very good performance on modern GPUs.

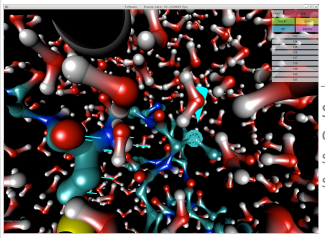






APPLICATIONS AND PERFORMANCE

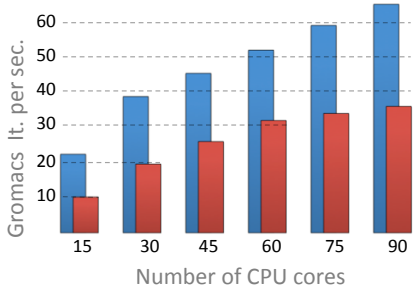
Interactive Molecular Dynamics



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.

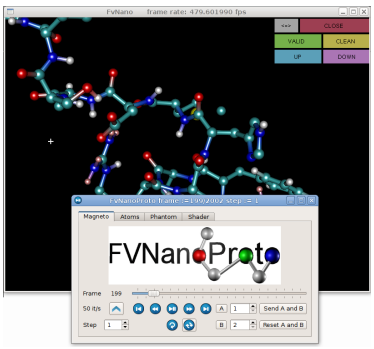
Screenshot of the molecular dynamics application. The cyan cone represent the position of the Phantom stylus and the lines show the force applied to the selected atoms

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.



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