GPU Acceleration in NAMD and VMD

Molecular Dynamics Simulation of MSCS (2.3 M atoms)
Alternatively we could use space-filling models to represent our structure such as CPK or VDW, the latter also giving us an idea of the volume and surface of the protein. Try applying these drawing methods and subsequently rotating the structure. Notice how these representations are still slower than we would like.

3.2. Introducing GPU-accelerated QuickSurf.

Now select the QuickSurf representation from the Drawing Method menu. Surprised by how fast the representation loaded? As you can see, QuickSurf lives up to its name by using the computational power of GPUs to calculate quickly the surface representation.

In addition to being fast, QuickSurf gives the user many useful options for controlling the representation. We can change the Radius Scale, Density Isovalue or Grid Spacing individually, or use the Resolution slider which will change them in tandem to give the desired resolution. Try adjusting the resolution and see how quickly the representation responds. This can be quite useful for changing on the fly from a high resolution, when you want to see detail, to a low resolution when you want the detail obscured.

Aside from faster rendering of surfaces than the traditional Surf and MSMS methods, QuickSurf also allows us to view an entire trajectory with a surface representation. Try playing the trajectory as you attempted before. Note that you can also adjust the resolution even while the trajectory is playing.

3.3. Usefulness of Surface Representations

Having a fast surface representation is great, but why might we want to visualize surfaces in the first place? As an example, look at the structure of the MscS in the QuickSurf. It consists of a seven-fold symmetric heptamer forming a balloon-like cytoplasmic domain attached to the transmembrane domain. There are several openings into the protein interior - the transmembrane channel, seven identical windows lining the balloon structure, and one at the C-terminus on the bottom of the balloon structure. Using a QuickSurf representation, you can quickly get a rough impression of how the sizes of these openings compare with one another. In particular, you can immediately tell that the C-terminus window is much smaller than the others. In fact, it is the only window which is impermeable to ions. The capability of running trajectories in QuickSurf makes it easy to see if windows are becoming wider or narrower, making it more apparent if, for example, a channel is opening or closing.

Next, we will modify the representation of different parts of the system to investigate how we can reduce the detail of certain components without removing them entirely.

1. Go to the Graphical Representation menu and create a selection “segname PA PB PC PD PE PF PG” in NewCartoon Drawing Method.
2. Create another representation of only “lipids” by clicking the ‘Create Rep’ button and typing ‘lipids’ into the Selected Atoms field.
3. Select QuickSurf for the lipids representation.
4. Under the “Draw Style” tab you can find an option named “Material”. Select “Transparent” for the lipids representation.
5. Tune the Resolution of QuickSurf to somewhere between 1.5 and 2. Notice how the lipid detail is reduced while still giving you a clear representation of the volume and overall shape of the membrane. Zoom into the lipid bilayer and notice how you can clearly see the transmembrane portion of the protein without losing the visualization of the lipids. An example of this view can be seen in Fig. 2.

While studying ion dynamics in the MscS system, you probably would not want to be encumbered by the fine details of lipid conformations. Using QuickSurf, you can reduce the detail level of the lipid bilayer. In general, the QuickSurf representation helps you to reduce the complexity of parts of the system without removing them entirely.

Another important aspect of visualization is discovery of features and phenomena which would otherwise have been hidden. The right representation can drastically change how you perceive the structure being modeled. For example, the capsid of the Satellite Tobacco Mosaic Virus (STMV) can be represented using QuickSurf to visualize the volume occupied by the proteins without unnecessary detail.

In addition to being visually appealing, when using QuickSurf we now notice that the capsid contains small holes in Fig. 3 which would have been much more difficult or even impossible to see with other representations.

QuickSurf Representation in VMD

Poor Man’s Anton GPU Accelerated aMD Simulation of Glucose-Galactose Binding Protein