High Quality Ray-Casting Visualisation on GPU:

From Small Molecules to Macromolecular Systems

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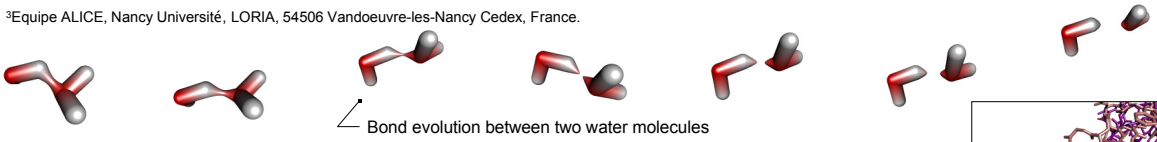
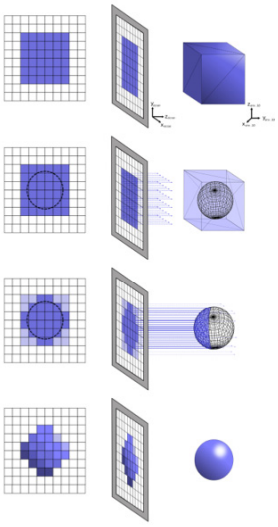


Bond evolution between two water molecules



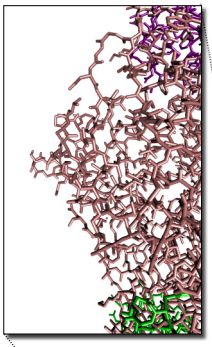
Ray-Casting Principle

GPU Ray-Casting Principle

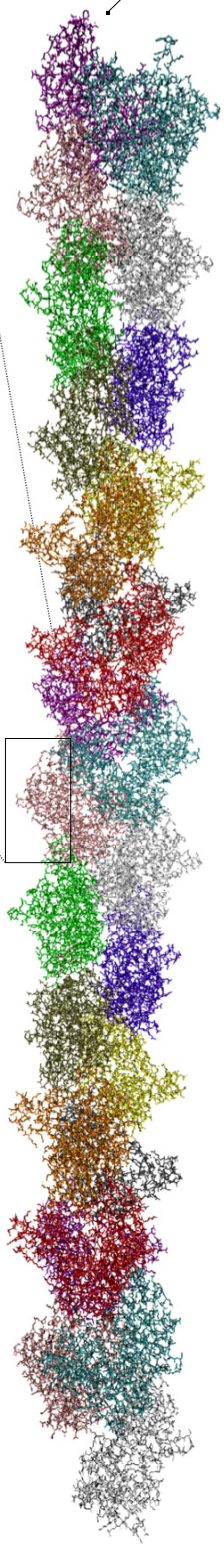
First, it is necessary to represent a simple triangulated envelop (the cube) using OpenGL. This envelop defines a set of pixels on the screen. For each pixel, we defined a ray with each screen pixel as origin and oriented orthogonally to the screen. In this envelop, we defined a surface equation (sphere) then we calculate the potential intersection between the rays and the surface. If the ray intersect the sphere origin pixel is kept otherwise the pixel is removed. Then, using sphere equation it is possible to define the surface lighting. The interest of this method is that, except cube creation, the entire process is calculated on GPU. There are several advantages:

1 - Create smooth surface with few triangles.
2 - Have a pixel accurate surface for all level of zoom (see ParM filament).
3 - Use GPU capabilities that accelerate calculations.

This principle has already been used to represent molecular surface [1] and is, here, used to represent different types of molecular metaphors.



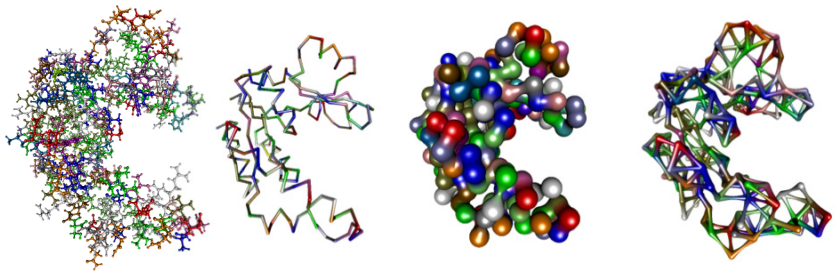
ParM filament *(~65,500 atoms)*



Molecular Representations

Classical representations as *Ball & Stick*, *Licorice* or *Van der Waals* are possible to depict with this method. We have also implemented a new representation that we named ***HyperBalls***. With this depiction, cylinders are replaced by hyperboloids that can smoothly connect the atom spheres. Interestingly, it is possible to adapt hyperboloids in order to depict bond evolution (see water molecules at the top) which is not possible using cylinders. Furthermore, this representation is well adapted to represent coarse grained or spring network models. This visualization could be also useful to represent ion coordination: to depict links between ion and other molecules or to define the cage that envelop the ion.

As presented on this poster, it is possible to color molecular metaphors by atom type, chain name, residue name, residue type (not shown) or other user defined colors.

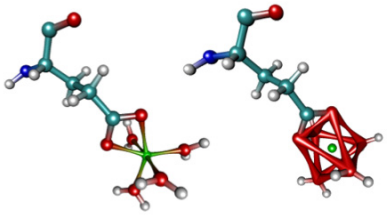


All atoms Ball & Stick ***Trace*** ***Coarse Grained Model*** ***Spring Network Model***

Macromolecular Systems Visualization

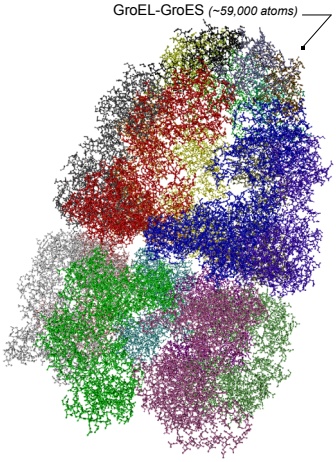
As explained before, this method is often more efficient to display interactively a huge number of atoms, indeed with a better image quality because there are less triangles to represent atoms or bonds. Thus, if we compare our results - in frame per second - with existing softwares (see table at the bottom), we can display the same molecules 5 to 6 times faster that can allow the user to move interactivelly the huge molecules that is impossible for tested molecular wiewer with frame rates under 10 fps.

To conclude, we present an efficient method to visualize interactively from small molecules to huge macromolecular systems with a high quality rendering. We hope that a molecular viewer based on this method will be freely available in the next months. For the moment, just ask for demos or videos.



Mg ion coordination visualizations

GroEL-GroES *(~59,000 atoms)*

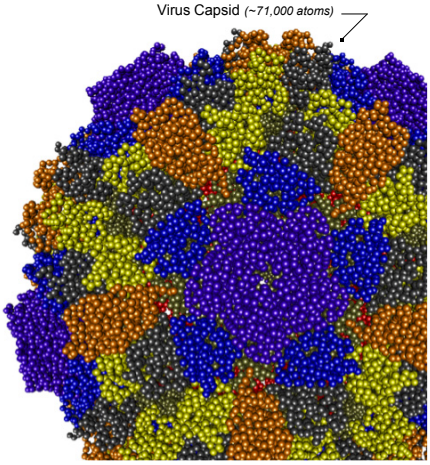


Comparison between Ray-Casting method and two molecular viewers

Molecule	VMD	MacPyMOL	Ray-Casting
GroEL-GroES (CPK)	4	3	28
ParM Filament (Licorice)	3	9	26
Virus Capsid (VdW)	4	3	21

In fps on MacOS 10.5.8 with an Nvidia GTX 285 graphic card (1024^2 screen)

Virus Capsid *(~71,000 atoms)*



References:

1. Chavent, M.; Levy, B.; Maigret, B. J Mol Graph Model 2008, 27(2), 209-216.

Acknowledgments: