HyperBalls on GPU: dynamic visualization of molecular structures

Scientific Visualization Accelerated by Graphics Processors

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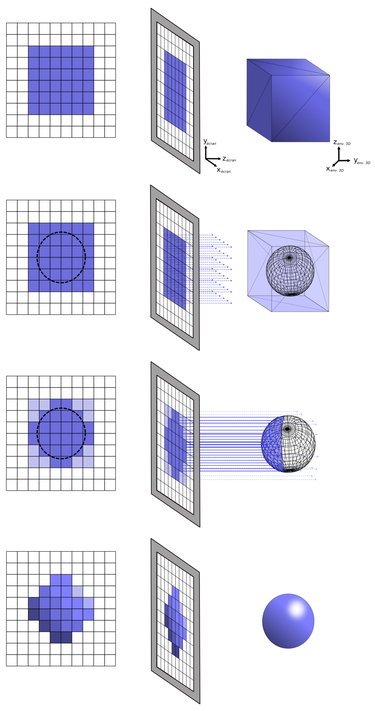
Project websites : ***http://hyperballs.sourceforge.net*** & ***http://exaviz.simlab.ibpc.fr***

Ray-casting on Graphics Processing Units (GPUs) opens new possibilities for molecular visualization [1]. We describe the implementation and calculation of diverse molecular representations such as licorice, ball & stick, spacefilling van der Waals spheres and approximated solvent accessible surfaces using GPUs. We introduce ***HyperBalls***, an improved ball & stick representation replacing tubes linking the atom spheres by hyperboloids that can smoothly connect them [2].

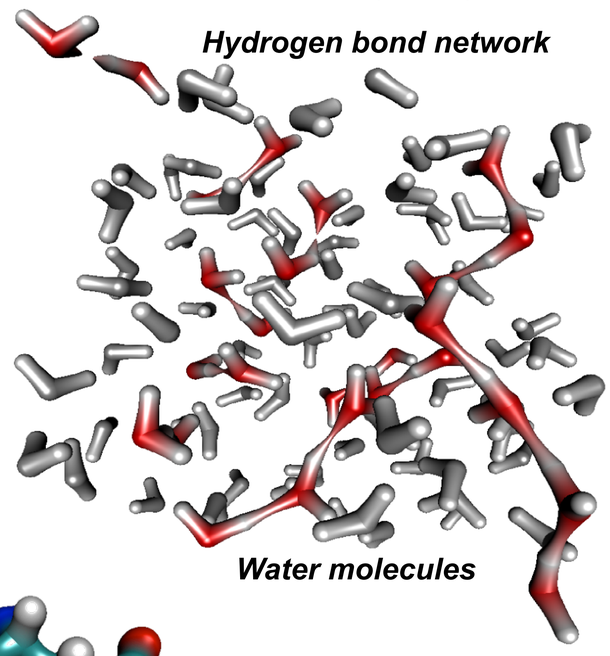


Ray-Casting Principle

GPU Ray-Casting Principle

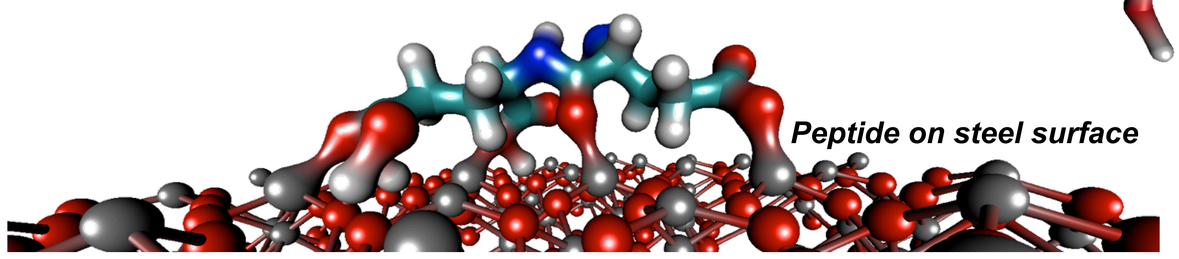
Consider rendering a sphere (Figure on the left). First, a simple triangulated envelope such as a cube is represented using OpenGL. It defines a set of pixels on the screen. For each pixel, we cast a ray from its origin. Within the envelope, we define a surface equation (sphere) and calculate intersections between rays and surface. If the ray intersects the sphere, the original pixel is kept, otherwise it is discarded. Using the equation of the sphere, we define surface lighting. Except for the initial creation of the cubes, the entire process is calculated on the GPU, providing several advantages:

1- Creation of a smooth surface with few triangles.
2- Pixel-accurate surface for all levels of zoom.
3- Accelerated calculations using GPU capabilities.



Hydrogen bond network

Water molecules

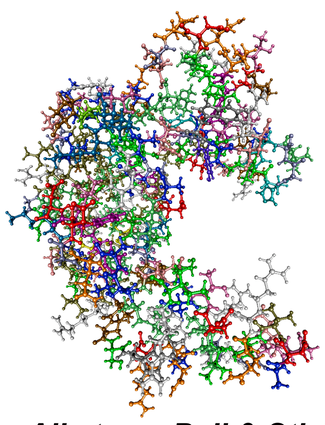


Peptide on steel surface

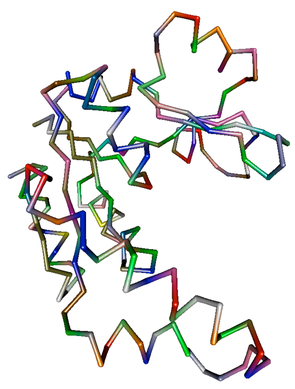
Molecular Representations

Classical ball & stick, licorice or Van der Waals representations are implemented with HyperBalls defining a single general algebraic equation. It is adapted for the ray-casting technique and well suited for execution on the GPU. It is possible to adapt the hyperboloids in order to depict dynamic bond evolution (see water network example at the top and alanate example below) which is not possible using cylinders. Furthermore, this representation can be adapted to represent coarse grained or spring network models (see picture to the left), systems biology "hairballs", experimental data, or to illustrate interactive molecular simulations. Another application is to represent ion coordination by depicting links between the ion and other molecules.

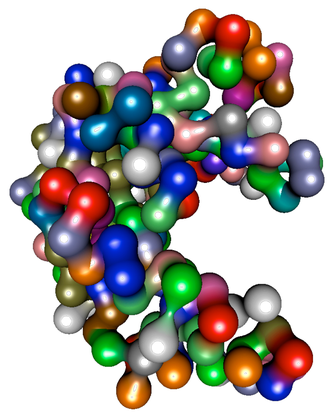
Molecular metaphors can be colored by atom type, chain name, residue name, residue type (not shown) or other user defined colors.



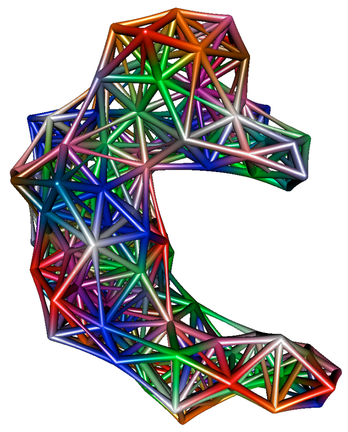
All atoms Ball & Stick



Trace

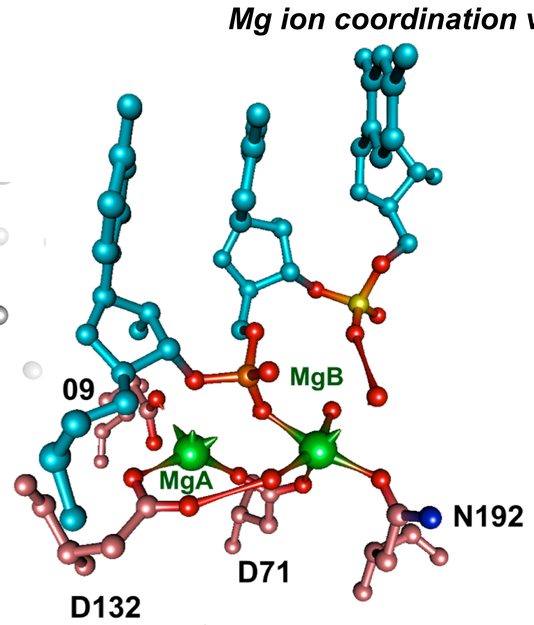


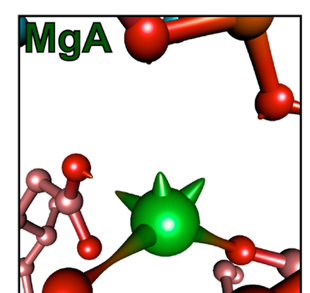
Coarse Grained Model

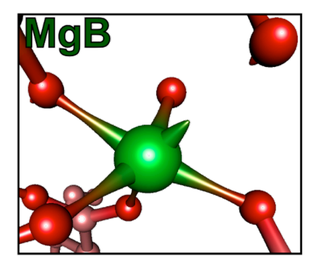


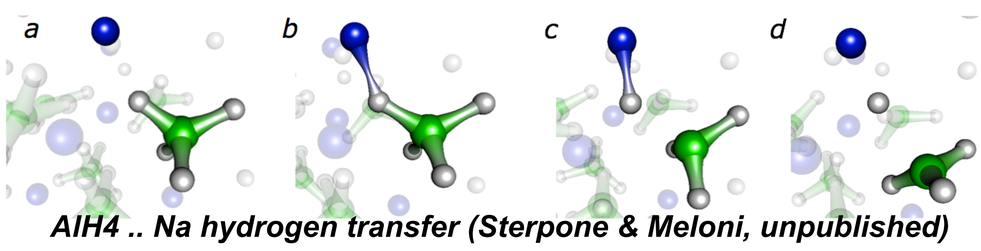
Spring Network Model

Mg ion coordination visualization

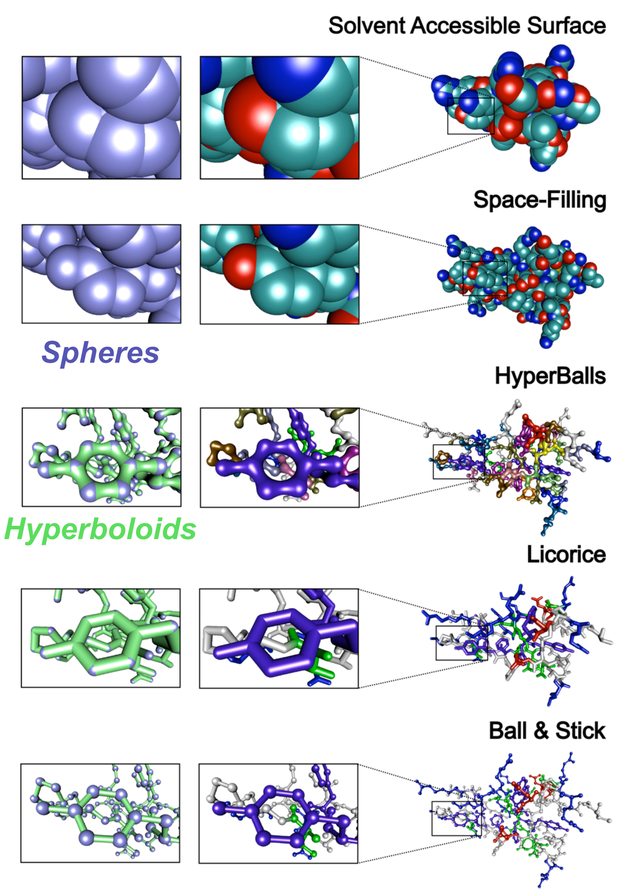








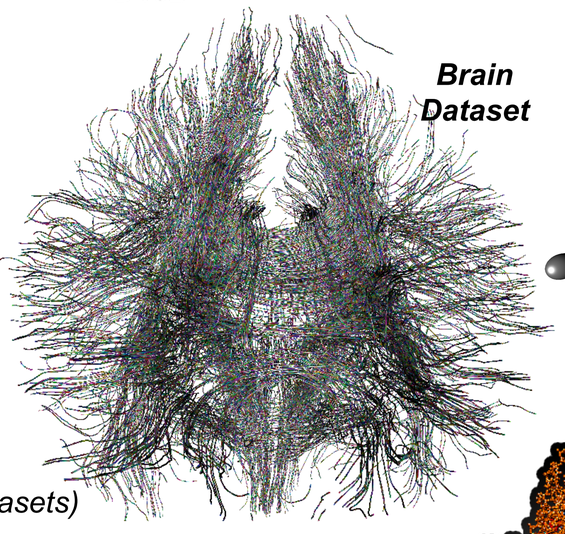
AlH4 .. Na hydrogen transfer (Sterpone & Meloni, unpublished)



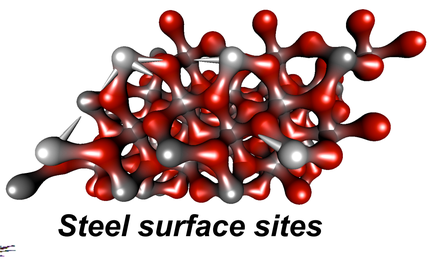
Macromolecular Systems Visualization

As explained above, this method is most efficient to interactively display a large number of atoms, achieving a high image quality because it requires less triangles to represent atoms or bonds. The gain in performance allows the user to interactively explore huge molecular structures. Furthermore, performance increases using new graphics card generations with exactly the same source code (see diagrams below).

To conclude, we present an efficient method to interactively visualize a broad range of molecules with a high-quality of rendering. MacOSX, Linux and Windows binaries and source code are available on the project website.

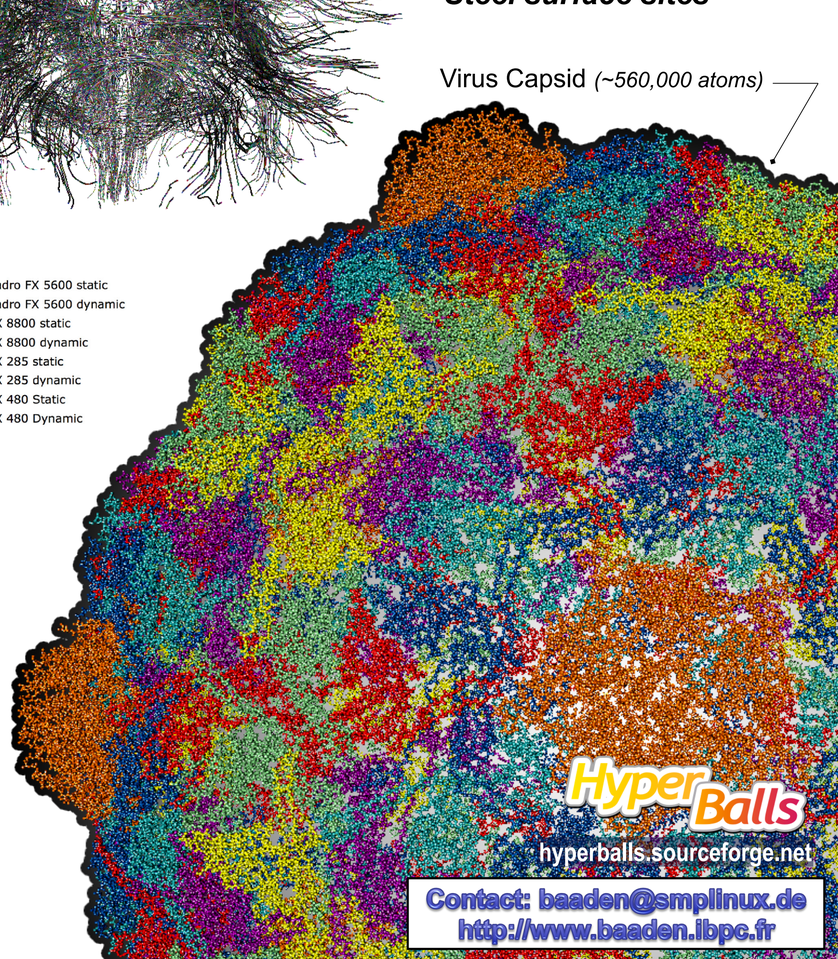


Brain Dataset

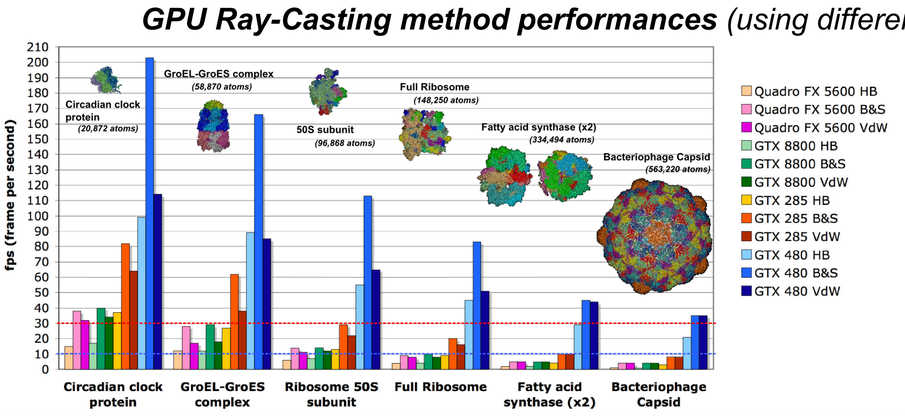


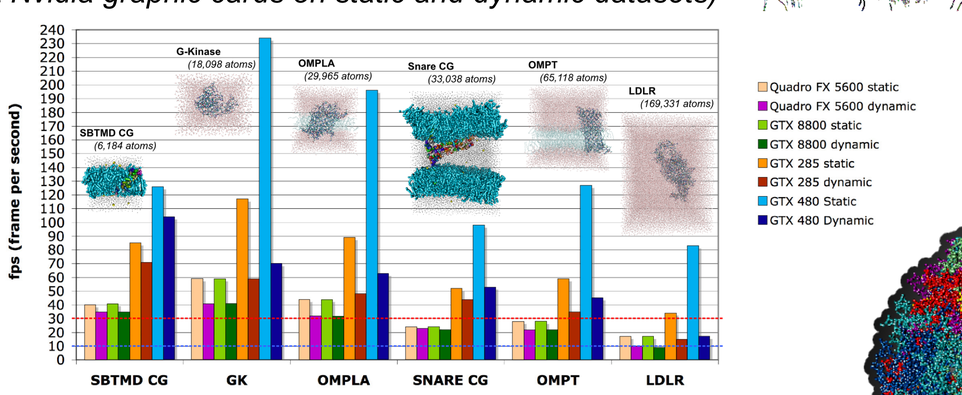
Steel surface sites

Virus Capsid *(~560,000 atoms)*



GPU Ray-Casting method performances *(using different Nvidia graphic cards on static and dynamic datasets)*





References:

1. M. Chavent, B. Levy, M. Krone, K. Bidmon, J. P. Nomine, T. Ertl and M. Baaden : "GPU-powered tools boost molecular visualization", *Briefings in Bioinformatics* 12, 2011, 689-701

2. M. Chavent, A. Vanel, A. Tek, B. Levy, S. Robert, B. Raffin and M. Baaden: "GPU-accelerated atom and dynamic bond visualization using HyperBalls, a unified algorithm for balls, sticks and hyperboloids", *J.Comput. Chem.*, 2011, 32, 2924.

Acknowledgments:

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