UnityMol: game engine-powered GPU-boosted molecular visualization

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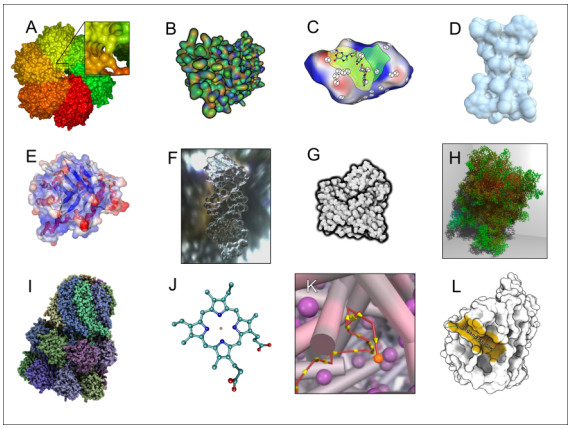
Computer science on its way to boost molecular visualization: a GPU story

In a recent review [1], we have taken a look at the latest contributions from the computer science field with the potential to revamp molecular visualization. The majority of these developments take advantage of new GPU programmability to revive well known molecular metaphors. We can cite a few examples. GPU-ray-casting creates on the fly metaphors with a pixel accurate quality, for example in molecular surfaces defined by Connolly (**A**), *metaballs* surfaces (**B**) or the molecular skin surface (**D**). Existing and new lighting effects can easily be implemented : see (**E**) for transparency mixed with GPU secondary structure visualization, (**F**) for high dynamic range rendering with a crystal effect, (**G**) for a halo effect, (**H**) for global shadowing; (**I**) for ambient occlusion. Finally, some methods are developed on CPU hardware to create new metaphors such as abstracted surfaces (**C**).

In less than a decade, substantial progress was achieved in molecular visualization. Many new programs draw benefit from the latest capabilities of graphics cards. Thanks to close collaboration between molecular scientists and visualization experts, prototypes of tools already exist in computer science labs and may soon become available to the whole scientific community (a current compilation can be found at http://www.baaden.ibpc.fr/projects/fvnano/gputools/).

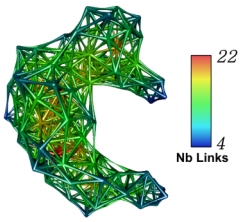


New and revived molecular metaphors. (**A-D**) several molecular surface representations: (**E-I**) illustrate different lighting effects to enhance molecular structure perception, (**J**) GPU ray casting Ball & Stick visualization of a heme group; (**K**) Depth of field blur and colour desaturation; (**L**) molecular annotation using text scaffolds. All details in [1].

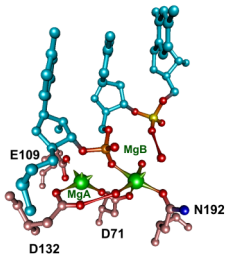
New Molecular Representations using GPU capabilities

Using GPU capabilities, we have designed a new molecular representation called ***HyperBalls*** [2]. With this depiction, cylinders can be replaced by hyperboloids that smoothly connect the atom spheres. Interestingly, it is possible to adapt the hyperboloids in order to depict dynamic bond evolution which is not possible using cylinders. Furthermore, this representation can be adapted to represent coarse grained or spring network models, or to illustrate asymmetric ion coordination (see pictures below).

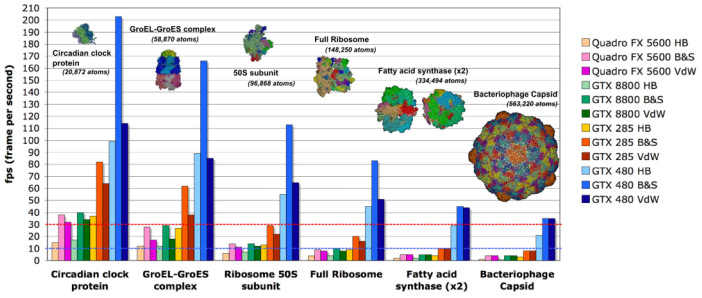
Coarse Grained Model



Spring Network Model



Ion Coordination



Performance of the HyperBalls GPU Ray-Casting method
(using different Nvidia graphics cards on a static view)

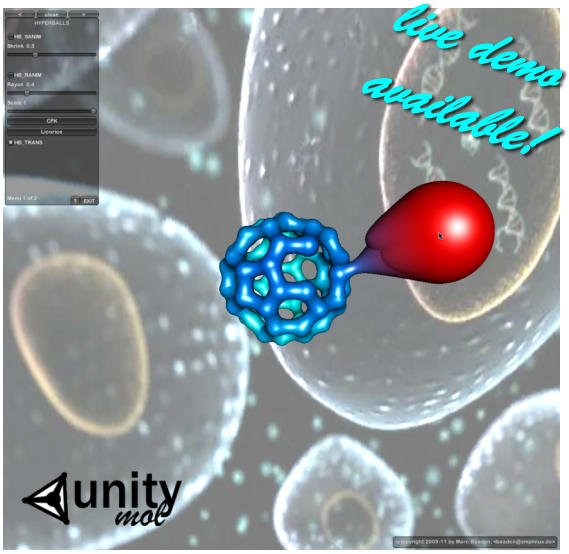
Performance of the HyperBalls method

The *HyperBalls* method is very efficient to interactively display a large number of atoms, achieving a high image quality because it requires less triangles to represent atoms or bonds. Thus, if we compare our performance results - measured in frames per second - with existing software, we manage to display the same molecules 5 to 45 times faster using our approach (compared to VMD or PyMol). Such a gain in performance enables the user to interactively explore huge molecular structures. Furthermore, performance increases using new graphics card generations with exactly the same source code (see performance diagram above).

UnityMol, a macromolecular viewer based on the Unity 3D game engine

The *Hyperballs* method is implemented in a software framework under active development. Here, we have built a prototype demonstrator using the Unity3D game engine (http://unity3d.com). The main advantage of this engine is the easiness to create appealing 3D environments with graphical user interfaces (as presented on the right). At this time, the rendering performance is limited, as some OpenGL and shader functionalities that are required for optimization are not exposed to the user. Unity 3D allows to quickly develop interactive tools to manipulate molecular structures and create prototypes that can be distributed as binary executables or webserver plugins on Mac and Windows platforms.

To conclude, we present an efficient method to interactively visualize a broad range of molecular structures, from small atomic systems to huge macromolecular assemblies with a high rendering quality. We strive to release a freely available version of this molecular viewer soon. Please check http://www.baaden.ibpc.fr/projects/fvnano regularly. At this time, demos or videos are available on demand.



Screenshot of the UnityMol molecular viewer prototype.

References:

1. M. Chavent, B. Levy, M. Krone, K. Bidmon, J. P. Nominé, T. Ertl, M. Baaden,
GPU-powered tools boost molecular visualization
Brief Bioinform (2011) doi: 10.1093/bib/bbq089 .
2. M. Chavent, A. Vanel, A. Tek, B. Levy, B. Raffin, S. Robert, M. Baaden,
GPU-accelerated atom and dynamic bond visualization using HyperBalls, a unified algorithm for balls, sticks and hyperboloids. Submitted

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