GPU-accelerated atom and dynamics bond visualization using HyperBalls: a unified algorithm for balls, sticks and hyperboloids

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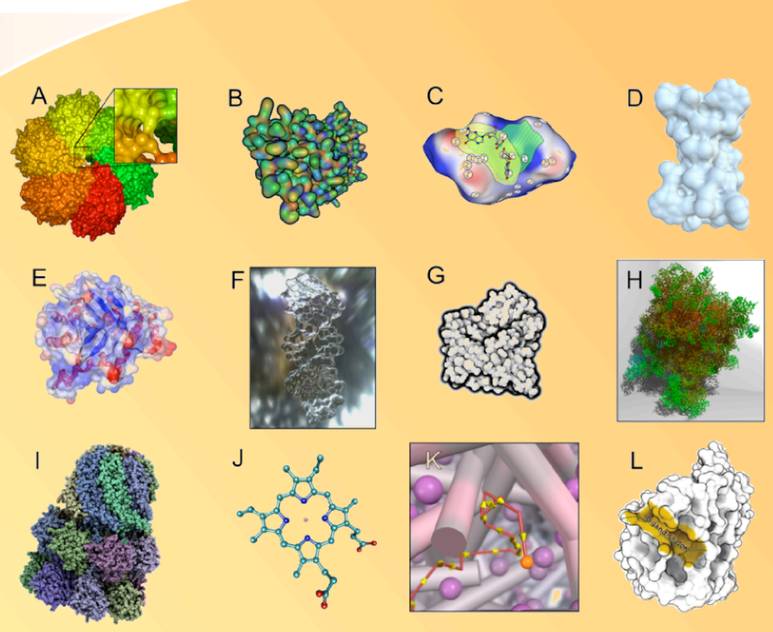


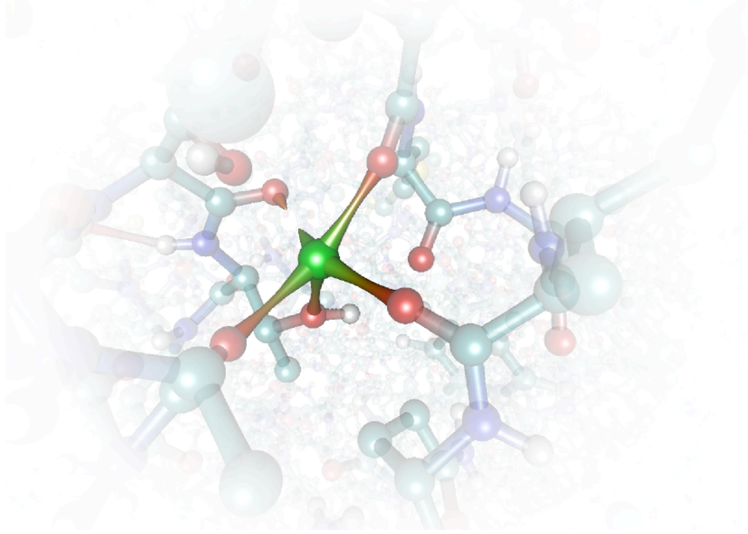
New and revived molecular metaphors. (**A-D**) several molecular surface representations: (**E-I**) illustrate different lighting effects to enhance molecular structure perception, (**J**) GPU ray casting Ball & Stick visualization of a heme group; (**K**) Depth of field blur and colour desaturation;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

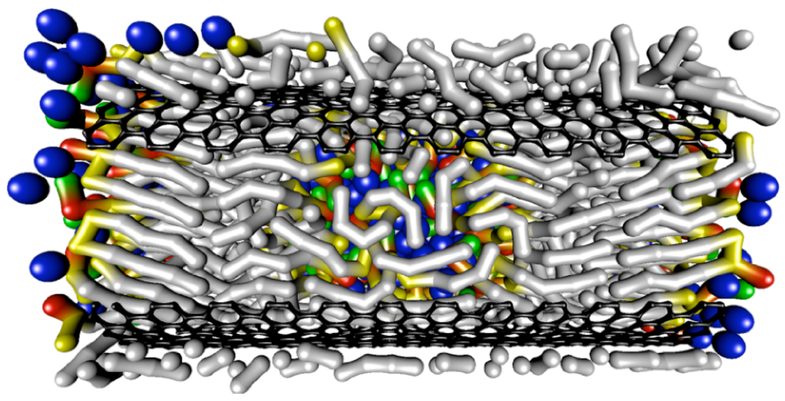
Computer Science to help molecular visualization: a GPU story

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

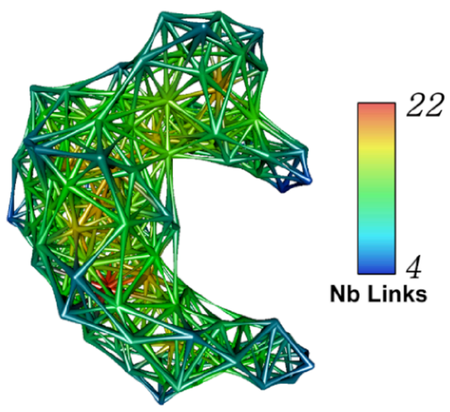
In less than a decade, substantial progress was achieved in molecular visualization. Many new programs draw benefit from the latest capabilities of graphics cards. Thanks to close collaboration between molecular scientists and visualization experts, prototypes of such virtual worlds already exist in computer scientists labs and may soon become available to the whole scientific community.

***Ion Coordination Model*[3]**





***Coarse Grained Model*[4]**



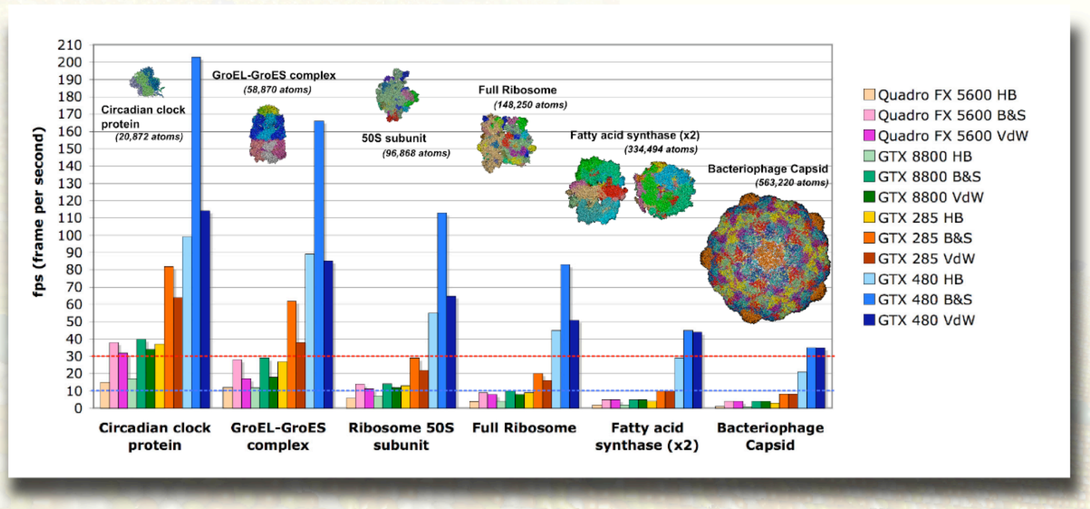
Spring Network Model

New Molecular Representations using GPU capabilities

Using GPU capabilities, we have designed a new representation that we named ***HyperBalls***. With this depiction, cylinders can be replaced by hyperboloids that can 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, spring network models (see opposite pictures) or ion coordination (see picture above). This method can also be used to represent mesoscale models as simplified proteins moving on a membrane[2] (see background image at the bottom).

Performance of this method:

This method is the 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. 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 can allow the user to interactively explore huge molecular structures. Furthermore, performances increases using new graphic cards generation with exactly the same source code (see performance diagram on right).



GPU Ray-Casting method performances *(using different Nvidia graphic cards)*

Conclusions :

To conclude, we present an efficient method to interactively visualize a broad range of molecules, from small atomic structures to huge macromolecular assemblies with a high-quality of rendering. We hope to be able to soon release a freely available version of this molecular viewer. Please, check http://hyperballs.sourceforge.net regularly. For the moment, demos and videos are available on demand. More details about pipeline and technical points on Marc Piuzzi poster and in a recently accepted article[5].

References:

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GPU-accelerated atom and dynamic bond visualization using HyperBalls, a unified algorithm for balls, sticks and hyperboloids, accepted in Journal of Computational Chemistry.

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