UnityMol: Interactive Scientific Visualization for Integrative Biology

Sébastien Doutreligne* Tristan Cragnolini† Samuela Pasquali‡ Philippe Derreumaux§
Marc Baaden¶

Lab. de Biochimie Théorique, CNRS UPR9080, Univ Paris Diderot, Sorbonne Paris Cité, 13 rue Pierre et Marie Curie, 75005, Paris, France

Abstract

A broad challenge facing scientists today is the availability of huge amounts of data from various sources. Computers are required to store, analyze, explore and represent these data in order to extract useful information. With UnityMol, we pursue the ambitious goal to create an interactive virtual laboratory enabling researchers in biology to visualize biomolecular systems, run simulations and interact with physical models and data. Visual effects can enrich the dynamic and immersive aspects. Ultimately, we want to combine an appealing visual feedback already in place with a set of analysis features to extract information about properties of the fascinating biomolecular systems under study.

Index Terms: I.6.6 [Simulation and Modeling]—Simulation Output Analysis; J.3 [Computer Applications]: Life and Medical Sciences—Biology and Genetics

1 Introduction

Nowadays, an increasing number of structures of molecular assemblies is available in a variety of databases. With the advances in experimental structure determinations, the size of these assemblies keeps expanding. Descriptive data from experimental measurements is abundant. Studying and exploring the high-dimensional set of properties of such huge structures is part of today's challenges to modern biology.

Visualization of molecular structures is commonly achieved by specialized software. UnityMol [5] in particular, uses a ray-casting technique called HyperBalls to render evolving atoms and bonds [1]. This innovative method is well suited for visualizing molecules moving according to accurate molecular simulations. In the last months, many features were added to turn UnityMol into an interactive virtual biology laboratory tuned for this purpose. Among them, we can cite the support of haptic interaction with the molecule, rendering on large, tiled high-resolution display walls and implementation of custom representations for RNA and sugar molecules.

Here, we present UnityMol's current features and, to some extent, our future developments for the interactive visualization and analysis of molecular and biological data.

2 Molecular Visualization in UnityMol

UnityMol includes both original and more traditional implementations of molecular graphics algorithms based on polygonal static and ray-casted dynamic rendering techniques. The former provide common tools for a static view of the system, the latter elegantly render dynamic biomolecular events such as the formation of bonds and interactions. Complex and large-scale data may be rendered on advanced displays such as the 33 megapixel 4,3x2,4 m display wall at Maison de la Simulation in Saclay. See Figure 1.

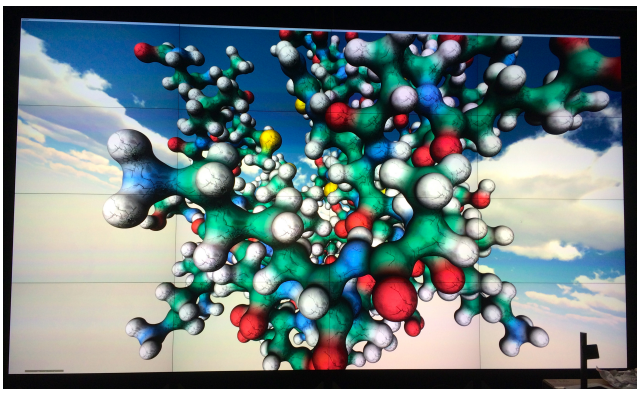

Figure 1: UnityMol running on a tiled display wall. The image is rendered accross a 4x4 display matrix at 7680 x 4320 pixel resolution. It represents the mono-heme ferrocytochrome c protein depicted in HyperBalls representation decorated with a cracked-stone lit sphere texture in front of a clouded sky skybox as background.

2.1 Surfaces, Secondary Structures, SugarRibbons and other Representations

UnityMol makes use of polygons to render molecular features, including among others molecular isosurfaces determined by marching cubes, secondary structures based on splines and a novel polysaccharide representation for complex sugar molecules. These representations are shown in Figure 2.

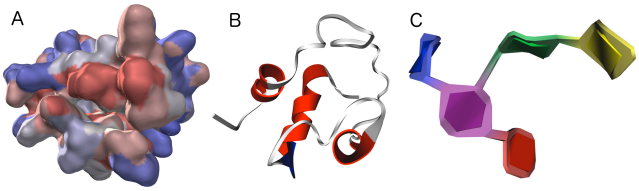

Figure 2: Representations of a hydrophobic surface of the ferrocytochrome c protein (A) and its helical secondary structures (B), SugarRibbons representation of the GLC-SIA-FUC-GAL-MAN pentaoligosaccharide courtesy of T. Tubiana and S. Pérez (C).

2.2 HyperBalls Representation

UnityMol comes with an HyperBalls GPU implementation. The heart of this ray-casting technique is the use of quadratic surface equations, perfectly compatible with a traditional rendering pipeline. Here, we successfully extend the representation to coarse-grained (CG) HiRE-RNA [6] models. Based on this coarse-grained

*e-mail:doutreligne@ibpc.fr
†e-mail:tristan.cragnolini@ibpc.fr
‡e-mail:samuela.pasquali@ibpc.fr
§e-mail:philippe.derreumaux@ibpc.fr
¶e-mail:baaden@smplinux.de

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model developed in the laboratory [2], nucleo-bases can be rendered as ellipsoids as shown in Figure 3. Visual feedback of molecular properties can be enhanced using a lit-spheres lighting pass.

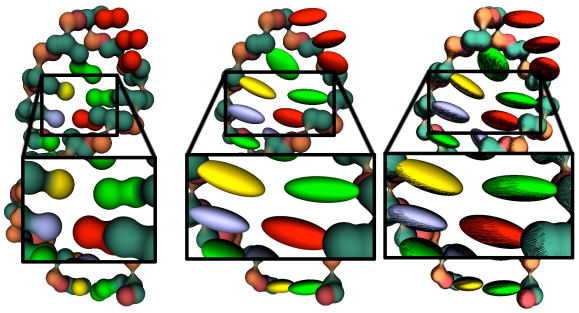

Figure 3: A coarse-grained HiRE-RNA model of a 22-Nucleotide Hairpin (1F9L). Left to right: HyperBall view, extension with ellipsoid base pairs and textured view mimicking hand-drawn shadows.

3 Live Simulation and Interaction

UnityMol has the ability to connect with molecular simulation software via the IMD network protocol. VRPN is used to support special devices such as an haptic arm and a 3D mouse.

3.1 Interactive Molecular Dynamics Simulation

UnityMol uses MDDriver, a light and generic framework for coupling molecular simulators with visualization software based on the IMD protocol [4]. Here, we focus on the coarse-grained, MDDriver-enhanced HiRE-RNA simulation engine. As a CG model, it provides an excellent compromise between simulation speed and biological fidelity, being in our experience more robust with respect to user interactions than computations carried out at an all-atom level. Enriched by special screen-space effects such as motion blur or glowing atoms, the underlying dynamic molecular behavior is highlighted visually.

3.2 Virtual Reality Enhanced Interactive Simulations

The interactive approach opens up perspectives to guide simulations via user input, within a dedicated graphical environment. Peripherals such as a 6 d.o.f. 3D mouse ease the navigation in the virtual space. The user can change the point of view intuitively, and focus on the relevant part. Haptic devices help to render accurate molecular models more real and tangible to the scientists. Hence, the user feels an immediate force feedback by a straightforward combination of molecular modeling and virtual reality leading to an intuitive understanding of the causal relationship between the theoretical model and its biologically relevant properties.

4 Interactive Unfolding of an RNA Hairpin

A typical biological application would be to stretch an RNA hairpin on two ends, controlling the successive detachment of its base pairs. When released, the structure may either progressively return to the initial hairpin state or feature a base shift. This numerical experiment provides insight into the hairpin's resilience, similarly to what can be probed experimentally with optical tweezers.

Figure 4 depicts a typical setup. The displayed screen is a montage exhibiting visualization features soon to be implemented, as described in section 5. A benchmark measuring the average FPS is displayed for five systems of increasing size.

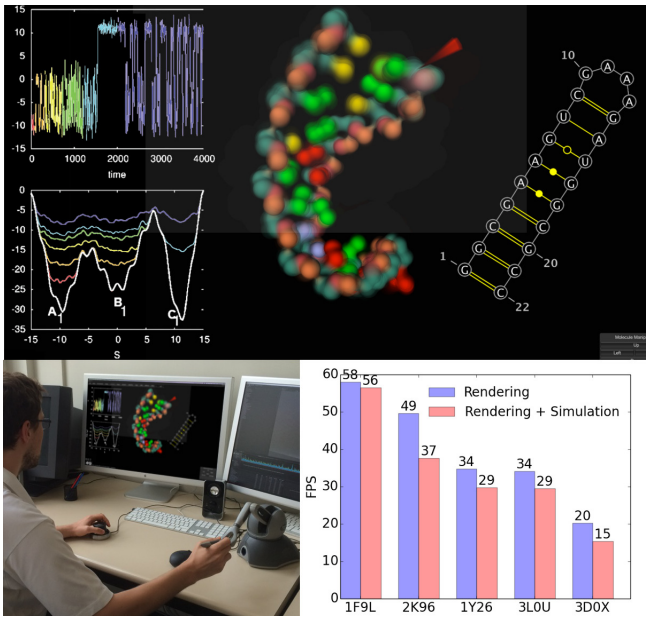

Figure 4: Photo montage of a typical workspace. The user moves the camera (left hand) and manipulates the 1F9L molecule in the center with the haptic arm (right hand). To the right, a 2D representation of the RNA molecule's secondary structure and hydrogen bonds is shown. To the left, a distance time series plot and an energy surface plot are depicted. Bottom right: benchmark for five RNA systems of 146, 303, 459, 475 and 1062 coarse-grain particles, respectively.

5 Upcoming Features and Future Work

Our current focus is on HiRE-RNA specific features such as the detection of hydrogen bonds in realtime. They will then be rendered in 3D as well as in two-dimensional schematic graphs of RNA molecules, commonly used in this scientific community. For this purpose, we couple UnityMol with VARNA, an image generator for RNA secondary structures [3]. We intend to add plotting functionalities to monitor the running simulation. We may watch the evolution of the mean distance between atoms, the number of weak bonds, the energy, etc., offering a visual dashboard for investigating molecular properties of biological systems.

6 Conclusion

We presented UnityMol as a platform for a full-blown virtual laboratory, featuring graphical representations of molecular data coupled with interactive visual analysis tools.

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