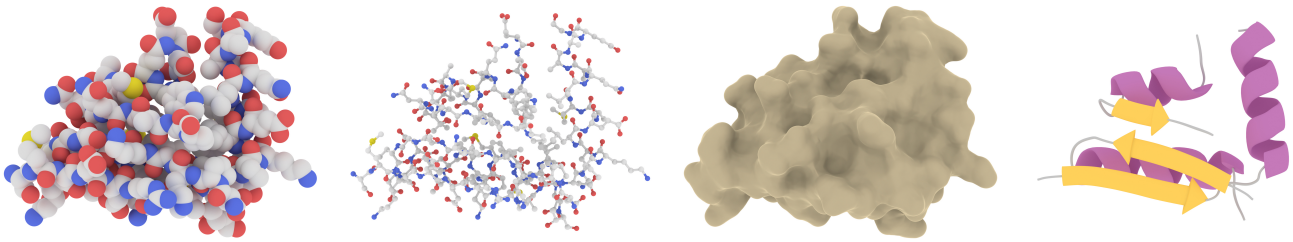
Software rasterization of large and complex molecular systems

1 Context

Interactive molecular visualization plays an essential role in structural biology, enabling to see the structure of molecules such as proteins or DNA. This insight helps the scientists to understand the interactions between molecules to design new drugs for instance [Ols18]. Molecules can be depicted in various ways, each providing specific information about their properties [KKF+17]. Figure 1 shows the geometric variety of representations that can be used.



(a) van der Waals (b) Ball-and-Stick (c) Solvent Excluded Surface (d) Cartoon

FIGURE 1 – Different representations of the same molecule.

With the development of computing resources, molecular simulations are getting larger, and can now contain over billion atoms [JND+19]. However, the interactive visualization of such complex scenes remains a very challenging task, so numerous works have been carried out to take more and more atoms into account.

This project falls within this context and aims to **enable the real-time visualization of large, all-atom molecular simulations on commodity hardware**. To achieve this, we will propose **new software rasterization methods**, specifically designed for the different existing molecular representations and their complex geometry.

As for classic 3D objects, all molecular representations can be described by a triangular mesh. However, in order to produce images of acceptable quality, many triangles are needed to define the geometry and have smooth surfaces. Even if GPUs are designed for fast triangle rendering, the number of required triangles is prohibitive for real-time visualization. To tackle this problem, molecules can be rendered using ray casting of implicit surfaces, reducing memory requirement while providing pixel-perfect rendering. This has been achieved for molecular representations composed of quadrics such as spheres and cylinders (*cf.* figures 1(a) and 1(b)) [RE05, TCM06], for surfaces (*cf.* figure 1(c)) [KBE09, PV12, RZK+19] as well as for secondary structures (*cf.* figure 1(d)) [LBLH19]. Nevertheless, these methods are not sufficient to enable real-time visualization at the scale we are targeting (*i.e.* from dozen of millions to billions of atoms).

Another way to speed up visualization is to reduce the number of primitives to be rendered. This can be achieved using level-of-detail representations [SKNV04] or occlusion culling techniques [GRDE10] for instance. Some works assume that large systems are often composed of re-

curring and static molecular subsystems, enabling to use instancing [LBH12, FKE13], to generate atoms on-the-fly [LMPSV14] or to cluster atoms into spheres in a preprocessing step [PJR+14]. Le Muzic *et al.* [LMAPV15] leveraged these works to propose « cellView », a tool capable of visualizing whole cell. In our case, we want to improve the raw rendering performance of molecules, considering each atom at its own position, so we cannot rely on this kind of assumptions.

Software rasterization is a rendering technique in computer graphics that processes and generates 2D images entirely through software, without relying on specialized hardware acceleration such as GPUs and their integrated graphics pipeline. This kind of technique was shown to be faster than the hardware pipeline for the first time by Liu *et al.*, for small triangles [LHLW10]. Several works have followed [LK11, PTSO15] and some complete pipeline implementations have been proposed [KKSS18, KB21]. However, none of these methods is really faster than the hardware pipeline under typical conditions. Software rasterization of 3D objects has received more attention recently with the release of the Unreal Engine 5 and its virtualized geometry method called « Nanite » [KSW21]. It consists in a hybrid software/hardware rasterization pipeline that achieves performance levels up to 3 times faster than a conventional approach. This performance suggests that software rasterization could be effectively adapted for other types of geometric primitives.

Software rasterization of point clouds has been shown to be faster than hardware one [GKLR13, SKW21]. Recently, Schütz *et al.* proposed a pipeline capable of rasterize up to two billions point at 60 frames per second on commodity hardware [SKW22].

For all these reasons, we are convinced that software rasterization could be a good candidate to enable real-time visualization of molecular simulations as complex as those carried out today.

The first goal of this project is to study how to accurately project to the image plane the complex shape of the geometric primitives associated to the different molecular representations :

1. Ball-and-Stick (*cf.* figure 1(b)), which is made up of spheres and cylinders ;
2. representations of the secondary structure such as Cartoon (*cf.* figure 1(d)) and its derivatives, which are composed of some kinds of ribbons that can be described by B-Splines ;
3. Solvent Excluded Surface (*cf.* figure 1(c)), which is divided into patches of implicit surfaces, as defined in [QS16, PMMM24].

The second goal is to design the whole pipeline itself. We will first provide a full CPU version, enabling our method to be used on computers not equipped with a GPU. In addition, it will also serve as a sandbox for proofs of concept. Then, we will tackle the high-performance GPGPU version of the pipeline, taking advantage of all the features of modern GPUs such as efficient intra-warp communication. We will need to carefully design our algorithms and data structures in order to maximize processing cores utilization while optimizing memory bandwidth. Setting up a streaming strategy with suitable data compression will be an important part of this work.

Over time, all the methods resulting from this project will be integrated in the open-source high-performance molecular visualization software VTX (`https://vtx.drugdesign.fr`), that we are developing in collaboration with other laboratories in France (GBCM - CNAM, Paris, LCT - Sorbonne Université, Paris).

2 Coordination

The scientific coordinator of the project is **Maxime MARIA**, assistant professor (maître de conférences) in computer sciences since 2019, at the XLIM Laboratory and the University of Limoges, France. He defended his PhD thesis on November 2016 which was entitled « Constrained Convex Space Partition for ray-based simulation » at the University of Poitiers, France. He is an expert in computer graphics, specialized in high-performance rendering, accelerating structures and parallel programming. He is now focusing is research on the visualization and simulation of complex molecular systems. In particular, he developed the core graphics engine of the high-performance molecular visualization software VTX.

The team working on the project also includes :

- Stéphane MERILLOU, Professor of computer science at the University of Limoges, XLIM Laboratory. Expert in computer graphics with research interests including aging and weathering, natural phenomena, physically-based rendering and molecular visualization.
- Matthieu MONTES, Professor at the Conservatoire National des Arts et Métiers Paris, GBCM Laboratory. Expert in structural biochemistry with research interests in molecular modeling, drug discovery and design, interactive simulation methods and computational geometry.

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