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# VTX: REAL-TIME HIGH-PERFORMANCE MOLECULAR STRUCTURE AND DYNAMICS VISUALIZATION SOFTWARE \*

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## ABSTRACT

**Summary:** VTX is a molecular visualization software capable to handle most molecular structures and dynamics trajectories file formats. It features a real-time high-performance molecular graphics engine, based on modern OpenGL, optimized for the visualization of massive molecular systems and molecular dynamics trajectories. VTX includes multiple interactive camera and user interaction features, notably free-fly navigation and a fully modular graphical user interface designed for increased usability. It allows the production of high-resolution images for presentations and posters with custom background. VTX design is focused on performance and usability for research, teaching and educative purposes.

**Availability and implementation:** VTX is open source and free for non commercial use. Builds for Windows and Ubuntu Linux are available at <http://vtx.drugdesign.fr>. The source code is available at <https://github.com/VTX-Molecular-Visualization>

**Keywords** molecular visualization, molecular graphics, usability, molecular modeling, molecular dynamics, high-performance computing, protein structure, structural biology

## 1 Introduction

Molecular visualization is a critical task usually performed by structural biologists and bioinformaticians to aid the different processes that are essential to understand structural molecular biology [1]. Following the recent advances in the determination of atomic resolution molecular structures and assemblies [2], in protein structure prediction [3, 4], and in the increased accessibility of molecular dynamics simulation [5, 6], there is a profusion of molecular structural biology data that is available to the scientific community. Due to the modern High-Performance Computing hardware and storage, the size of the simulated systems [7, 8, 9] with molecular dynamics has dramatically increased and the storage, analysis and interactive visualization of the resulting data can become problematic for currently available molecular visualization systems such as PyMol [10], VMD [11] or Chimera-X [12].

Here, we present VTX, an opensource molecular visualization software. VTX is optimized to handle efficiently and in real-time the big data in molecular simulations notably by including a meshless high performance molecular graphics engine coupled with a minimalistic task-oriented GUI to maximize the usability for non-expert users. VTX uses the chemfiles library to read and write molecular data which handles most widely used molecular structures and trajectories file formats. VTX includes various representations and rendering options and provides different tools such as structural alignment and distance/angle measurement for interactive analysis of massive molecular scenes. It is free and open source for non commercial use and available on linux and windows at <http://vtx.drugdesign.fr> and <https://github.com/VTX-Molecular-Visualization>

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## 2 Methods

### Molecular Graphics Engine

Thanks to adapted data structures and rendering algorithms, VTX is designed for the real-time visualization of very large molecular systems, composed of several millions atoms, on a consumer laptop. A molecule is defined by the position of its atoms, their corresponding radius and connectivity.

#### *Meshless Representations:*

Most of VTX representations are described implicitly, without using a triangular mesh (sticks, ball and sticks, Van der Waals, Solvent Accessible Surface). These meshless representations allow impostor-based techniques in the rendering engine [13]. For each primitive, a simple quad is rasterized. Then, ray-casting is used to evaluate the implicit equation of the primitive and display the final shape. This allows fast and pixel perfect rendering while reducing the memory consumption and bandwidth usage which is essential to handle large molecular structure or dynamics data.

**Cartoon and SES representations:** The Cartoon representation is generated on-the-fly and displayed with adaptive level-of-detail (LOD) method using tessellation shaders[14].The Solvent Excluded Surface is computed following a discrete approach, similarly to [15] and the resulting surface is extracted via marching cubes [16].

**High Quality Rendering:** VTX aims to enhance the user's visual analysis experience in real-time by providing high-quality rendering (Figure 1B). The use of meshless representations in VTX results in a pixel-perfect display quality. Additionally, VTX offers various rendering options to improve the perception of details and enable the creation of visually appealing illustrations. The deferred rendering approach allows for the implementation of various post-processing techniques, including shading (flat, matte, glossy, toon), ambient occlusion, fog, outline, and anti-aliasing. These techniques can enhance the visual perception of molecular shape and improve overall image quality. VTX offers an image export feature that allows to produce an image of the displayed molecular scene with a resolution up to 8K and a custom background with user-defined transparency. When dealing with dynamic data (such as MD trajectories), ambient occlusion rendering cannot be pre-computed. In VTX, we use a deferred shading graphics pipeline to compute lighting on surfaces and apply screen-space post-processes that allows to produce high-quality rendering in real time [17].

### Improved user experience

**Camera modes:** VTX disposes of an interactive camera system controllable via the keyboard and/or mouse that includes different modes: 1. trackball and 2. free-fly. The trackball mode is the classical camera available in molecular visualization software where the camera revolves around a fixed focus point. This allows the user to rotate the view around the object of interest. The first-person free-fly navigation mode allows the user to fully control the movement of the camera. This mode is similar to the first-person perspective in video games where the user can move freely in the 3D space. It has notably been used in UDock [18, 19] and in the multiscale molecular rendering tool CellVIEW [20]

**Keyboard controls:** Using a trackpad to navigate in 3D molecular scenes can be challenging because it may not provide the same level of precision and control as a mouse. This can make it difficult to perform precise tasks such as rotating, zooming, and panning the view. VTX provides alternative navigation controls using keyboard bindings to make it easier to use with a trackpad and to complement the mouse for the freefly navigation mode.

**Customizable Graphical User Interface (GUI):** The GUI of VTX enables to create customizable presets of combined displays and representations that can be saved and easily accessed. The different dockable windows of the software can be moved, resized, and arranged according to the user's preferences, allowing for a customizable workspace. It also includes quick access to the most frequently used commands in the 3D visualization window through the use of clearly labeled buttons.

### File formats compatibility

The Chemfiles library [21] is used to handle diverse file formats for molecular structures (including PDB, mol2, mmCIF and MMTF) and molecular dynamics trajectories (including dcd, xtc and arc). While mmCIF is the preferred format in VTX for molecular data as its structure is well adapted for very large molecular structures and assemblies, a direct download access to the PDB [22] is provided through the use of the PDB API.

### Implementation

VTX is written in C++, with modern OpenGL for hardware-accelerated rendering and the Qt [23] framework for its graphical user interface (GUI).

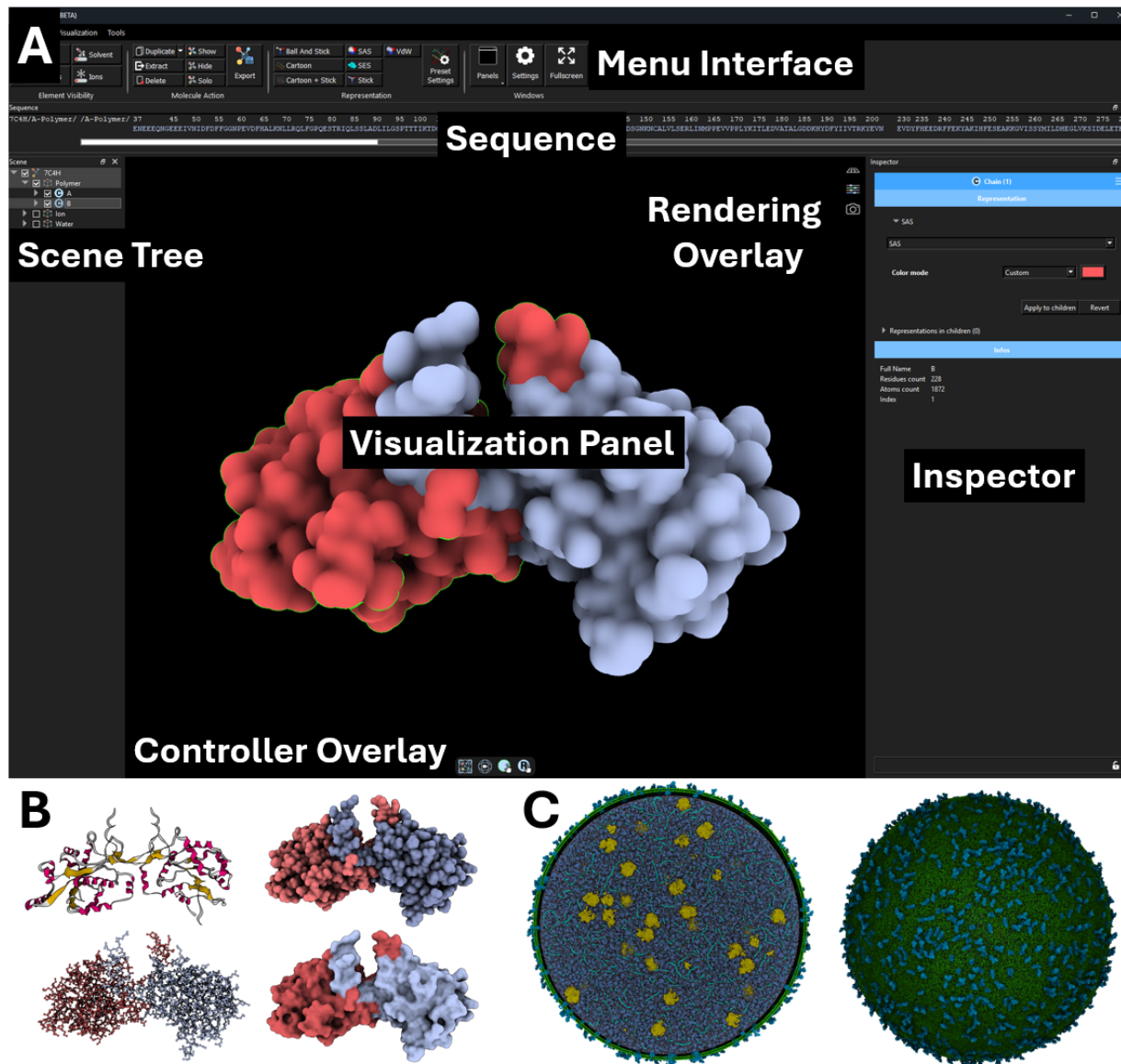


Figure 1: **A.** Illustration of the VTX GUI organized with different dockable panels. The *Scene Tree* panel contains and allows the selection of all the objects present in the scene, such as molecules, labels and viewpoints. The *Sequence* panel displays and allows the selection of the sequence of each biomolecule, while the *Visualization Panel* allows the selection, observation, and manipulation of their 3D structure. Frequently used options for manipulation and rendering are directly accessible in the visualization panel through the use of button overlays. When an object is selected in the scene, detailed information about the loaded object, additionally loaded trajectories and chosen representations are available in the *Inspector* panel. The *Console* panel displays all logs. **B.** Different molecular representations available in VTX (*Saccharomyces Cerevisiae* BCP1, PDB id : 7C4H) Cartoon (upper left), Van der Waals (upper right), balls and sticks (bottom left), Solvent Excluded Surface (bottom right) **C.** Illustration of the coarse-grained whole mycoplasma cell model from [8] with (left) and without (right) clipping. Martini beads are displayed as surface and flat color (membrane lipids in green, membrane proteins in blue, ribosomes in yellow, chromosome in light blue, cytoplasmic proteins in dark blue).

## Operation

VTX operates on computers with a graphics processing unit (GPU) that supports OpenGL 4.5. The software is compatible with Windows 10 and subsequent versions, as well as Ubuntu Linux versions 20 and higher

## Use case

The VTX GUI is organized as presented in Figure 1A. Molecular structure and trajectories can be loaded using the *open* button from the file menu or directly downloaded from the PDB with their accession number. For ease of use, molecular trajectories can be loaded with a right click onto an already loaded molecular object in the scene tree.

As illustrated in Figure 1C, due to its new generation molecular graphics engine, VTX is highly scalable and allows the rendering in real time of massive molecular systems (100+ million Martini beads) on a consumer laptop with a NVIDIA RTX2080m.

VTX also includes different functions in the *tools* menu tab for distance and angle measurements, as well as structural alignment using the CE method [24].

The session state, including the user's organization of the VTX workspace, can be saved and exported. High resolution illustrations with or without background can be generated with the *snapshot* function.

## Conclusion and perspectives

VTX is a molecular visualization software designed to provide: 1. a high-quality real time rendering of large molecular systems (several hundred million atoms on a consumer laptop) 2. a comfortable user experience with intuitive controls and tools and 3. a wide compatibility with most molecular structures and trajectories file formats and a high-quality image export feature allowing to produce up to 8K-resolution images with custom background for posters and presentations. Future versions will include real-time analytical SES [25], high-end real-time ambient occlusion, offline ray-tracer for high-quality illustrations and movies rendering, python-like command binding. VTX is open source and free for non commercial use.

## Data and software availability

### Software availability

VTX is open source and free for non commercial use under the VTX consortium license. Builds for Windows and Linux are available at <http://vtx.drugdesign.fr>. The source code is available at <https://github.com/VTX-Molecular-Visualization>.

## 3 Competing interests

No competing interest is declared.

## 4 Author contributions statement

MMa, SG and MMo designed the software; MMA developed the first version of the rendering engine. MMA, SG, ND, CPH, VG, VL, JL, YN contributed to the code; ND, JL and GL designed the interface; MMA, VG and MMo wrote the manuscript; MMA, VG, JPP, NL, SM, GL and MMo reviewed the manuscript

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