Interactive visual exploration of large flexible multi-component molecular complexes

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Abstract

While molecular visualization software has advanced over the years, today, most tools still operate on individual molecular structures with little facility to manipulate large multi-component complexes, or depict molecular flexibility. We extend and accelerate 3D image-based rendering via programmable graphics units to provide an order of magnitude speedup over traditional triangle-based rendering. Additionally, by employing a biochemically-sensitive level-of-detail hierarchy, we communicate appropriate molecular volume occupancy and shape while dramatically reducing the visual clutter that normally inhibits higher-level spatial comprehension. The hierarchical, image based rendering also allows dynamically-computed molecular properties data (e.g. electrostatics potential) to be mapped onto the molecular surface, tying molecular structure to molecular function. The collection of these techniques have been encapsulated in an interactive molecular exploration tool we call TexMol (short for Texture Molecular viewer), which supports simultaneous volumetric and structural rendering and synchronized multi-viewing.

CR Categories: I.3.4 [Computer Graphics]: Graphics Utilities—Application packages; I.3.5 [Computer Graphics]: Computational Geometry and Object Modeling—Hierarchy and geometric transformations

Keywords: molecular visualization, computer graphics, image-based rendering, texture-based rendering, imposter rendering, volume rendering, level of detail, hierarchy, multiresolution, synchronous view

1 Introduction

Visualization of large molecules – particularly of protein and RNA structures – has become an increasingly important tool in biological research. Previous work has focused on efficient rendering for single-component, static molecules, which is becoming increasingly restricted in light of the increasing demand for more complex, dynamic visualization and representation. We present TexMol (short for Texture Molecular Viewer), an interactive molecular exploration package created in response to the increasing visualization requirements of the biology community.

To efficiently represent dynamic and flexible molecules, TexMol uses an internal representation called the Flexible Chain Complex (FCC). The FCC provides a robust, dynamic representation of flexibility that is augmented with a biochemically-sensitive hierarchy for level-of-detail optimizations.

Besides high visualizer functionality, TexMol delivers rapid, accurate rendering via various novel applications of texture-based rendering techniques for structural and for volumetric representations. For the field of structural representation (e.g. CPK, ball-and-stick model), recent advances in programmable graphics hardware have opened the door for texture-based (a.k.a. imposter) techniques that greatly reduces geometric complexity while preserving, and in some cases improving the visual fidelity of the generated image. The level-of-detail hierarchy allows for static and dynamic multiresolution, which reduces the visual clutter that often accompanies atom-level visualization while still maintaining biochemical structural information, such as residue-level grouping. Combined with the level-of-detail hierarchy, texture-based rendering allows TexMol to render large and previously intractable molecules.

TexMol also supports efficient volumetric visualization via texture-based techniques. By combining rendering modes, the visualizer can either map volumetric data onto the structural model of the molecule or it can juxtapose multiple volume sets and structure models concurrently. In both cases, the resulting visualization ties molecular structure to molecular function in an elucidating manner

We will first summarize related work in Section 2. Section 3 explains the internal representation of the molecule and its properties. Section 4 provides an overview of rapid imposter-based rendering nad describes TexMol's specific imposter algorithms. Section 6 summarizes performance measurements. Finally, we discuss our conclusions and ideas for future work in Section 7.

2 Related Work

Molecular Modeling and Rendering Numerous modeling schemes have been used to represent and display molecules and their properties in computers [Leach 1996]. Some models which are structural in nature include the Stick model, the Ball-and-Stick model, the Wire-Frame model and the Cartoon model. All these in fact are different visual representation of an underlying hierarchical skeletal model of the positions of atoms, bonds, chains, and residues in the molecule. Hence, structural models aim mainly at representing the primary, secondary, tertiary and quaternary geometric structures of the molecule. Many visualization systems such as RasMol, PyMol, VMD & JMV, MidasPlus, PMV, and Rasayan

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