Computers & Graphics 52 (2015) 62–71

Contents lists available at ScienceDirect

Computers & Graphics

journal homepage: www.elsevier.com/locate/cag

Technical Section

View-dependent level-of-detail abstraction for interactive atomistic visualization of biological structures ☆

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ARTICLE INFO

Article history:
Received 2 February 2015
Received in revised form
17 June 2015
Accepted 23 June 2015
Available online 14 July 2015

Keywords:
Level of detail
Clustering
Space error metric
Scientific visualization
Biological structures

ABSTRACT

The visualization of biological structures is a challenging task because it requires rendering millions to billions of atoms in real time. In this paper, we propose a view-dependent approach by which a large biological scene can be visualized interactively. In this scheme, we first extract several levels of building blocks of biological structures from a molecular abstraction based on hierarchical clustering. We then define a volume-based distance metric for the clustering process to reduce "inflation" error and propose a quantitative error metric for the object space error evaluation. Finally, we utilize an adaptive screen-space level-of-detail selection with the error metric at run time. Empirical results demonstrate that our molecular hierarchical abstraction method achieves high quality rendering results and performs better than other existing methods. Moreover, our result also shows that the view-dependent approach provides valid results in a large biological scene with more than 10 billion elements.

1. Introduction

Biologists have started to rely significantly on biological visualization and simulation to understand the molecular machinery of life. In coarse-grained (the so-called mesoscopic) particle-based simulations, biological structures often consist of millions to billions of atoms. Real-time atomistic rendering is a challenging task as it incorporates a large number of particles.

On the other hand, biological data sets consist of only a few individual molecules with a large number of instances. To take advantage of the repetitive nature, many instances can be rendered using the same building block. To reduce the geometric complexity of rendering a biological scene, hierarchical geometrical representations are often used to simplify unnecessary model details. Particle-based data reduction and data simplification are the main approaches of molecular hierarchical abstraction. As the work of Parulek et al. [1] shows that fast hierarchical clustering (FHC) [2] is an available simplification approach to abstract various levels of detail. However, the utilization of FHC brings two major limitations. First, it is difficult to find the most suitable parameters for evaluating the clustering method. Second, utilizing hierarchical abstraction is necessary to perform sequential clustering.

For interactively rendering large biological scenes, we need to overcome these limitations. Our main focus lies in the hierarchical geometry abstraction of large biomolecular data sets on PCs. The contributions of this paper can be summarized as follows:

- With a volume-based distance metric (VDM), we propose sophisticated molecular hierarchical representations by hierarchical clustering. Our distance metric achieves a better quality of clustering and an outstanding performance.
- We define an approximate metric to quantitatively evaluate the object space error, and we also use this error metric for adaptive LOD selection.

Our main motivation is to help scientists to see the big biological structure interactively in a level-of-detail way, and achieve atomistic visualizations of mesoscopic simulations which can have above billions of atoms. We organize the rest of the paper as follows. After presenting the related works on large biological visualization (Section 2), we illustrate the framework of our view-dependent macromolecule rendering (Section 3). We present the

☆This article was recommended for publication by Stefan Bruckner.

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http://dx.doi.org/10.1016/j.cag.2015.06.008
0097-8493/

details of molecular hierarchical representation (Section 4), in which surface representation (Section 4.1) and the hierarchical clustering method (Section 4.2) are explained. Consequently, we present the view-dependent LOD rendering algorithm (Section 5), including our object space error metric (Section 5.1) and LOD selection algorithm (Section 5.2). A discussion of the results is provided in Section 6. Section 7 provides discussion and outlines the limitations of our work. Conclusions and future work are presented in Section 8.

2. Related work

Because data sets consist of a large number of particles, some parallel visualization systems, such as ParaView and VMD, are developed for clusters of workstations. As noted in the Introduction section, our main focus is hierarchical geometry abstraction of large biomolecular data sets on current desktop PCs. Our approach builds on several aspects of previous work on large biological structure visualization, in particular with respect to molecular surface representation, LOD approaches and molecule assembling.

2.1. Molecular surface representation

There are several types of molecular surface representations. The Van der Waals (vdW) surface [3] is the first and simplest definition. As a space-filling model, vdW surface defines each atom as a sphere around the atom's centre. However, vdW surface can scarcely show the actual accessible region of the molecule with the surrounding solvent. In 1977, Richards [4] defined the Solvent Accessible Surface (SAS) by the centre of a spherical probe that rolls over the vdW surface of the molecule. In 1978, Greer et al. [5] proposed the Solvent Excluded Surface (SES). The SES is the topological boundary of the union of all possible probe spheres that do not intersect any atom of the molecule. As a type of molecular surface, the SES has served many purposes including visualization, analysis of molecular interactions and the study of cavities in molecular structures. Consisting only of spheres, surface computation is easier for the vdW and SAS but not for the SES. To achieve interactivity with the scene, biologists sacrifice a bit of information provided by SES and investigate molecules with blobby Gauss kernel representations [6]. Recently, Lindow et al. [7] gave a more sophisticated molecule surface called Ligand Excluded Surface (LES). The LES is defined by replacing the probe sphere with a full geometry of the ligand defined by the arrangement of its vdW spheres. It represents a more accurate approximation of the regions accessible to the ligand than the SES does. However, it is obvious that a new computational challenge is associated with the calculation of the LES.

With advancements in GPU hardware, direct particle-based rendering techniques, in particular the ray-casting method, are usually adopted for molecular surface visualization. Tarini et al. [8] used ambient occlusion as an approximation of global illumination as well as additional techniques, such as halos, to improve the perception of the spatial structure of large balls-and-sticks and space-fill models. Krone et al. [9] presented a GPU ray-casting technique for visualizing the SES of proteins and achieved interactive frame rates even for long protein trajectories, for which conventional methods based on precomputation are not applicable. Furthermore, to accelerate the construction and the rendering of the SES and the molecular skin surface, Lindow et al. [10] proposed several improvements to reduce the update times for displaying these molecular surfaces. Chavent et al. [11] introduced an improved ball-and-stick representation called HyperBalls replacing tubes and linking the atom spheres by hyperboloids that can smoothly connect them. Parulek et al. [12] utilized the theory of implicit surfaces and their CSG operations to compose the implicit function representing the molecular surface locally.

In addition, some optimizations were proposed for fast rendering. Kanamori et al. [13] applied depth peeling to fast ray casting for a large number of metaballs. Krone et al. [14] proposed a parallel contour-buildup algorithm for the molecular surface to meet computational demand. By extending Tarini et al. [8]'s work, Szecsi et al. [15] replaced depth peeling with gathering per-pixel fragment lists in a single pass, which scaled well for a large number of particles.

2.2. Level-of-detail approaches

The level-of-detail technique for real-time large scene rendering has a long history with many studies in various research fields. For example, Pajarola et al. [16] surveyed semi-regular multiresolution models for interactive terrain rendering, and Balsa Rodriguez et al. [17] conducted a survey of compressed GPU-based direct volume rendering. Common types of large data sets, such as cosmological and surfel data are originally particle-based. Because of structure irregularity, particle data require more attention in the LOD process. In view of a hierarchical quantization scheme for particle coordinates and rules for generating coarse particle distributions, Fraedrich et al. [18] proposed a visually continuous LOD particle representation. The amount of cosmological data is significantly reduced while maintaining a user-defined screen space error. Introducing polygon-implicit error metrics, Kanai et al. [19] described an efficient error-driven method for the hierarchical approximation of implicit surfaces from polygonal meshes. Similarly, Clasen et al. [20] presented a quasi-continuous level of detail method that is based on an image error metric to minimize the visual error by successive simplifications using ellipsoids and lines. Because the source ellipsoids is organized in a Delaunay tetrahedralization, it may cost more time in the preprocess step for LOD modelling.

Unlike cosmological particle data sets or surfel, the atom is usually represented not as a point but as a sphere. Relative to the distance between two atoms, the atom radius is considerable. In 2014, Muzic et al. [21] exploited the primary task of tessellation shader to lower the number of the tessellation levels according to an increasing camera distance. The vertex shader decides on the number of atoms to be generated. By skipping more and more atoms and scaling the radius of remaining atoms, the hierarchical abstraction is built dynamically on the GPU. Parulek et al. [1] provided a visualization approach that improved the overall rendering performance by utilizing an LOD concept applied via hierarchical clustering. Inspired by Parulek's work, we use hierarchical clustering for hierarchical abstraction. However, without error evaluation, the LOD selection mainly depends on the distance from eye to rendering target in Parulek's and Muzic's work [1,21]. Despite its simplicity, as Luebke et al. [22] indicated, distance-based LOD may lead to more obvious popping effects under certain conditions. A more precise and adaptive LOD selection is important to solve this problem. Therefore, we propose an object space error metric for dynamic view-dependent LOD of biological scenes.

In addition, it is possible to make use of some biological rules for molecular hierarchical abstraction. Lampe et al. [23] presented a two-level rendering approach that enabled visualization of slow dynamics of large protein assemblies. In their research, residues are represented as higher level building blocks of protein. For data simplification, we also pay attention to residues as a particular level. Zwan et al. [24] provided a method to visualize continuous transition between different stages of structural abstraction as well as aspects of spatial perception and illustrativeness.