

Visibility Equalizers for Molecular Visualization

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Abstract

In scientific illustration and visualization, cutaway views are often employed as an effective technique for occlusion management in densely packed scenes. We propose a novel data-centric method for authoring cutaway illustrations of mesoscopic biological models. In contrast to the existing cutaway algorithms, we take advantage of the specific nature of the biological models. These models consist of thousands of instances that are distributed across a comparably smaller number of different molecular types. Our method constitutes a two stage process. In the first step, culling objects are placed in the scene, creating a cutaway visualization of the model. During this process, histograms inform the user about the instance visibility distribution of each individual molecular type in the scene. In the second step, the visibility of each molecular type is fine-tuned through these histograms, which at this point act as interactive visibility equalizers. The technique has been evaluated by domain experts in scientific illustration.

Categories and Subject Descriptors (according to ACM CCS): I.3.3 [Computer Graphics]: Picture/Image Generation—Viewing algorithms

1. Introduction

Biology is an emerging field where the state of the current knowledge changes extremely quickly. New discoveries have to be communicated to a large variety of audiences. Since these discoveries often happen on the microscopic level and they are not directly observable in sufficient detail, illustration is the only way how to communicate them.

Traditional pipeline of the scientific illustrators starts with the collection of data and knowledge gathering. Afterwards, they make sketches, in which specific regions of the illustrated objects are uncovered. For this, occlusion management techniques are necessary. Oftentimes, *cutaway views* are employed, where specific parts of the scene are removed from the illustration, so that internal structures become visible. When new knowledge is discovered, the conceptual layout of the illustration might break down and the whole pro-

cess has to start from the beginning. Therefore, the duration of this process counts in months or even years.

With the rapid changes to the knowledge in the field of biology, it is necessary to adapt the traditional illustration pipeline so that the new data can be easily plugged in and the resulting illustrations can be updated accordingly in a very short time period. Virtual models of cells and other mesoscale molecular structures can be utilized for this purposes. These models can be created with tools such as *cellPack* [JAAA*15] and the knowledge from the field of integrative structural biology. The models consist of multiple instances of several molecular types. The instances are densely packed within predefined compartments according to the biology knowledge.

The mesoscale biological models represent the geometry of microorganisms, cells, or even viruses at atomic resolution. However, simply displaying such models does not guarantee an adequate view of internal structures, which are often necessary to communicate through an illustration. This is due to the high density of the molecular instances present in the models. To solve this problem, visualization techniques need to be developed which reproduce the occlusion management methods used in traditional illustration.

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Currently, occlusion management in virtual models is carried out by placing culling objects in the scene, which remove specified parts of the displayed model. During this process, the illustrator does not have a good overview of what instances have been already removed, and which molecular types are still sufficiently represented in the scene. The illustrator has to continuously check the modelled scene against the gathered data and tediously confirm whether all the necessary molecular types are still present.

To alleviate this process, we present our first contribution. During the process of placing the culling objects in the scene, we display *visibility histograms* of the molecular types, which immediately reveal which of them are underrepresented or overrepresented. By looking at the visibility histograms, which are continuously updated, the illustrator is able to modify the placement of the culling objects in such a way that every molecular type is adequately represented in the scene. This is the coarse-level of the visibility specification process.

In illustration, fine-level visibility specification is often utilized as well. To communicate the biology knowledge well, the illustrations have to sometimes display molecular instances which would be impossible to specify with the simple culling objects, such as cutting planes. An example is shown in Figure 1. Figure 1a shows an illustration of a HIV virus. In Figure 1b, a cutting plane is used to reveal internal structures of the virus - the capsid containing the RNA. Some of the glycoproteins (yellow molecules) are left in the illustration to communicate their presence on the surface of the virus particle. In particular, those glycoproteins which are not occluding the object of interest, were chosen to be kept in the illustration providing the contextual information. In this way, the main components of the virus particle can be illustrated in a single image.

The process of fine-tuning the visibility is extremely time-consuming, as the illustrator has to pick individual molecular instances to be reintroduced or removed from the scene. This might be done to control the under and overrepresentation of some of the molecular types, removing instances occluding important aspects of the model, suggesting shapes, etc.

To significantly speed up the fine-level visibility specification, we propose our second contribution - *visibility equalizers*. To explain how the visibility equalizers are used to speed up the process of fine-tuning the visibility in molecular models, we use the metaphor of hi-fi sound reproduction. In the hi-fi sound systems, volume control is the basic tool for adjusting the output sound uniformly on all frequencies. This corresponds with the coarse-level visibility specification through culling objects in the molecular scenes, where all molecular types are uniformly removed from the culled regions. However, hi-fi sound system allow users to fine-tune the sound through *equalizers*. With equalizers, the volume of each individual frequency band can be adjusted separately to achieve desired sound during the reproduction. To achieve

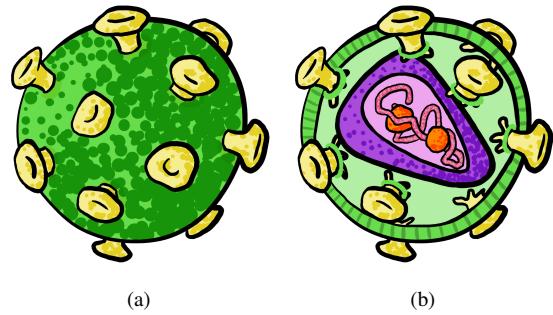


Figure 1: (a) Illustration of a HIV virus. Here, outside membrane of the virus particle is visible. (b) Cutaway view of the HIV virus. Despite the cutaway, some of the glycoproteins (yellow molecules) are kept in the view to provide adequate context.

similar level of control for the visibility in the molecular models, we make the visibility histograms interactive. Individual bins of the histograms can be dragged to increase or decrease visibility of the individual molecular types within the scene, given the specified culling objects. The interactive element effectively turns the visibility histograms into visibility equalizers for the molecular models.

2. Related Work

[VKG05] [BHW^{*}07] [BF08] [LRA^{*}07] [LHV12] [MAPV15]

3. Overview

3.1. Design Principles for Cutaway Illustrations

[here we write what principles are there, and how is our system fulfilling them] [LHV12]

There are several issues with using cutaway views in illustrations. First one is that it has to be clear from the visual representation of the cut that the given part of the object has been removed artificially for the sake of illustration. Otherwise the viewers might believe that the hole created by the cut is in fact inherent part of the object. This is commonly solved by using specific shapes of the cuts which significantly differ from the shapes naturally occurring within the object (e.g., using circular cut on object which only have straight edges).

Another issue is that the information about the part of the object that is being cut away is lost. In technical illustration, this issue is often circumvented by displaying contours of the cutaway part of the object. Alternatively, small portions of the cutaway parts can be reintroduced into the scene. These graphical elements are not occluding the objects of interest,

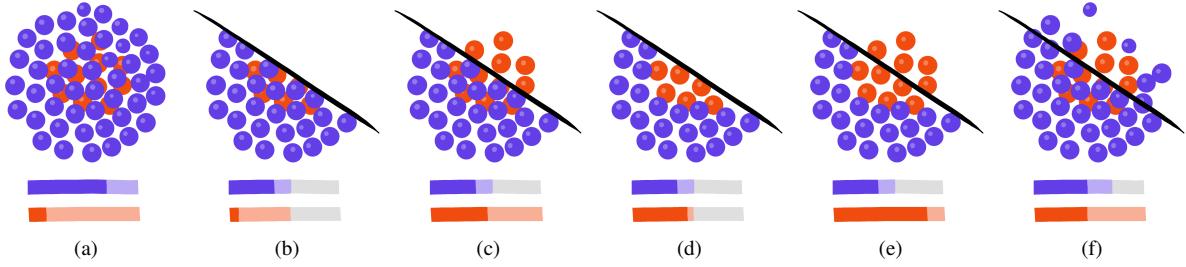


Figure 2: Visibility Equalizers.

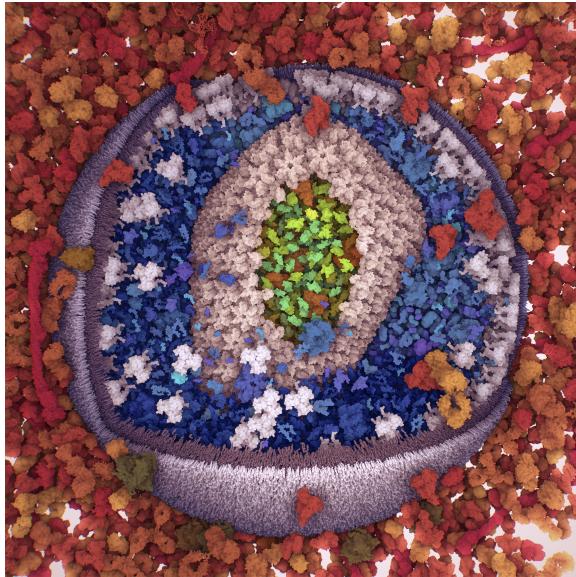


Figure 3: An illustration of the HIV virus in the blood serum utilizing cutaways created with our approach.

but at the same time they help to convey the overall shape of the cutaway part.

4. Fuzzy Cutaways

5. Equalizing Visibility

6. Evaluation

7. Results and Discussion

8. Conclusions

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