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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 molecular level and they are not directly observable in sufficient detail, illustration is the only way how to communicate them.

Traditional pipeline of the scientific illustration starts with the collection of data and knowledge gathering. Afterwards, illustrators 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 form the organism model in 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 process 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 3D models of cells and other mesoscale molecular structures can be utilized for this purposes. These models can be created with tools that procedurally assemble individual molecules into large complexes and into entire systems such as bacterial organisms. An example of such a tool is *cellPack* [JAAA*15]. These tools take individual molecular ingredients, as well as shapes of compartments where the instances of these ingredients are populated, as input. Output of these tools are 3D models consisting of multiple instances of several molecular ingredients. The instances are densely packed within the predefined compartments. The shape of the compartments is designed by the domain experts in biology.

The mesoscale biological models represent the structure of microorganisms, cells, or even viruses at atomic resolution. However, simply displaying such models does not guar-

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antee an adequate view of internal structures. These structures are often the key for the function of the organism, and should be therefore shown in an illustration. The internal structures are occluded because of 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.

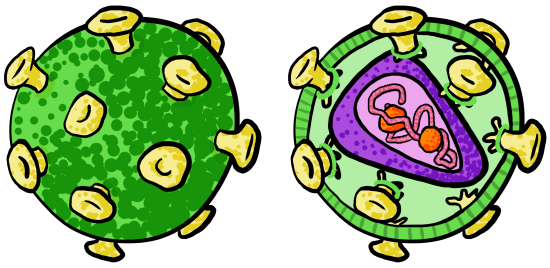
Currently, occlusion management in mesoscale virtual models is carried out by placing clipping objects in the scene, which remove specified parts of the displayed model. During this process, the illustrator does not have a good overview of what instances have been already removed, and which molecular 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 clipping objects in the 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 clipping 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 traditional 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 clipping 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 in our approach utilizing 3D virtual models, 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



(a) (b)

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.

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 clipping objects in the molecular scenes, where all molecular types are uniformly removed from the clipped regions. However, hi-fi sound system allows 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 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 clipping objects. The interactive element effectively turns the visibility histograms into visibility equalizers for the molecular models.

Our main contributions are:

- A new workflow for illustrator-authored cutaway illustrations from mesoscale 3D structural models.
- A new visual metaphor of visibility equalizers with which allows users to fine tune the cut-away design so that visibility is distributed among the molecular types as desired by the illustrator.

2. Related Work

[overview of related areas]

2.1. Visualization of Molecular Structures

[MAPV15] -this work is based on cell view

-refs from cellview papers

-only short overview

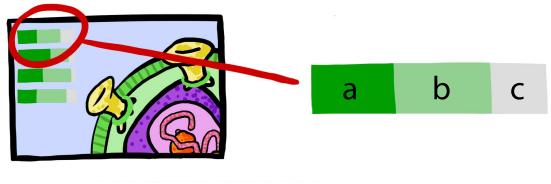


Figure 2: Visual representation of the visibility equalizers.

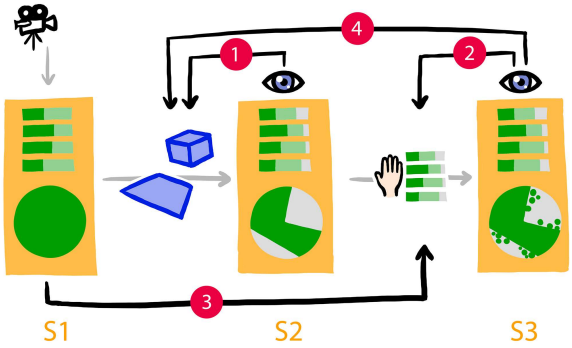


Figure 3: User-centric overview of our method.

2.2. Occlusion Management

- overview of techniques based on Elmqvist survey - motivation for occlusion handling - argumentation for different techniques
- cutaway techniques: volumetric & polygon approaches
- other techniques: transparency,..

[VKG05] [BHW*07] [BF08] [LRA*07] [LHV12]

2.3. Visual Steering

[coffey et al - design by dragging]

[additional refs from coffey paper]

3. Overview

In this work, we focus on visualization and illustration of 3D models of mesoscale molecular structures, such as cells or viruses. We utilize *cellView* [MAPV15] tool for both representation and rendering of our 3D scenes. These scenes can consist up to billions of individual atoms, each belonging to one of the molecular ingredients.

The visual representation of the visibility equalizers is illustrated in Figure 2. The equalizers are represented by three stacked histograms, where each histogram bin represents single molecular ingredients. Each bin is a stack of three values, denoted as *a*, *b*, and *c*. The part *a* shows the number of visible instances of the given ingredient. The part *b* shows the number of instances not removed by clipping,

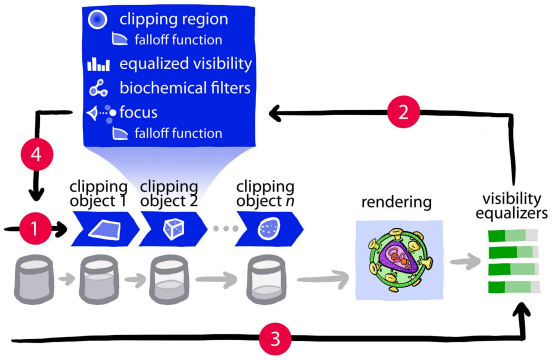


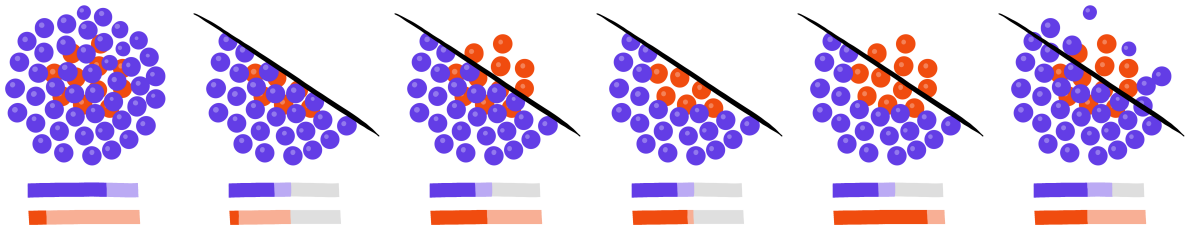
Figure 4: Technical pipeline of our method.

but not visible due to occlusion. The part *c* represents the number of instances which has been clipped away.

Figure 3 illustrates how our method is utilized by users. The method can show the data in one of three states, denoted as *S1*, *S2*, and *S3*. In the state *S1*, the data are shown without any clipping applied. The visibility equalizers are already shown, displaying the proportion of visible and occluded instances of the individual ingredients, however the user does not interact with them yet. In this state, the user can specify the viewing direction, which might modify the values displayed by the visibility equalizers.

In the state *S2*, parts of the scene are removed. The user can switch from the state *S1* to the state *S2* by placing and manipulating cutting objects. These are represented as distance functions, of which zero level-sets are used as the clipping criteria. The visibility equalizers now also show the portion of the molecular instnaces, which has been clipped away. So far, the clipping has been done in a deterministic manner.

At this point, the user can use the information displayed by the visibility equalizers to steer the iterative process of the placement and the manipulation of the clipping objects (path 1). However, at this point there is also the possibility of the direct interaction with the visibility equalizers. The values in the individual bins of the displayed histograms can be dragged in order to increase or decrease the number of clipped instances of certain ingredients, switching to the state *S3*. This is carried out in a probabilistic manner. If the number of clipped-away instances is decreased, the probability that an instance passing a clipping test will be removed continuously decreases from 100% to 0%. On the other hand, if the the number of clipped-away instances is increased, the probability of instances which do not pass the clipping test being removed from the scene continuously increases from 0% to 100%.



(a) (b) (c) (d) (e) (f)

Figure 5: Visibility Equalizers.

4. Workflow

5. Object-Space Clipping

Cull object define how instances of a given ingredient type shall be clipped.

Each cull object stores clip parameters for each ingredient types.

Additionally cut parameters can be associated with a geometrical shape that localize the clipping in the domain.

Cull objects are applied in serial as shown in figure XX.

Internally, for each cull object and for each single instance, we first determine the region of the clipping and then we determine if the instance shall be clipped according the cull object parameters.

Moreover, additional gradient parameters allows for advanced customization of the clipping region.

5.1. Clip Parameters

For each cut object and for each ingredient type, there are two basic parameters that allow to control the visibility of entire sets of instances based on their type.

When associated with geometrical shape, the cull object will only influence thee sub-region of the domain, defined by the geometry, e.g, plane, sphere, cone...

It is worth mentioning that in case no shape is associated with the cull object, the clipping will be evaluated to the entire domain.

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The first parameter is the percentage of visible elements of a given type.

We refer to this value as object-space clip probability.

This value allows us to control the degree of fuzziness of the clipping.

The other filtering parameters are related to biochemical properties and allows us to control the clipping based on the mass and/or quantity of given ingredient types.

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Prior to the rendering, after localizing the clip region, each single instance is evaluated in order to determine if it shall be clipped.

First is applied the filtering based on the clip probability on the ingredient type.

For each instance, we compare a uniformly distributed random number with the clip probability.

If the random number is higher than the probability, the instance is marked as culled, and will not be rendered.

The random number is initially set for each individual instance and remain the same for each re-evaluation of the clipping, in order to guaranty reproducibility of the scene.

Secondly, instances are filtered according to their biochemical properties, for each cut object and each ingredient types the user defines range values for the both quantities and molecular weight.

Instances whose properties lie outside on these ranges are marked as culled and will not be rendered.

5.2. Analytical Distance Evaluation

At the very beginning of the process, for each instance, the first task of the clipping is to determine whether an instance is located in the sub-region defined by the geometry.

Our system currently supports the following set of primitive shapes (plane, cube, sphere, cylinder and cone)

To evaluate if an instance lies inside or outside the clip object region, we compute the signed distance between the instance bounding sphere and the closest point on the region surface.

Although the supported shapes have a simple topology, it may still be computationally expensive, using a mesh-based representation, to evaluate the signed distance of a large number of instances.

Indeed, using a triangle-based discretization for the shape

would imply evaluating the signed distance between the instances and every single triangle of the mesh.

To accelerate the computation we solve the problem analytically using a mathematical description of the 3D signed distance field (SDF).

Using such representation instead reduces the problem of evaluating the signed distance to solving trivial equations.

It is also possible to apply traditional transform operations to the distance field, such as translation, rotation and scaling.

The clipping region can also be reversed by inverting the result of the signed distance function, offering users flexibility.

Using, for instance, a spherical shape, the clip region would be set to the inside of the sphere by default, while in inverted mode it would correspond to the inside of the sphere.

5.3. Gradient

We provide additional options to gradually remove instances given a geometrical shape.

The purpose is to facilitate the removal of instances, primarily for illustration purposes.

TODO PMINDEK: Talk about gradient clipping here

6. Visibility Histograms

To provide a clear overview of the scene properties, we display histograms for each ingredient type that indicate information about their visibility.

By default we chose to show three ranges in each histogram. The section of the histogram (dark green region) shows the percentage of instances that are currently visible on the screen. The entire green section (dark & light green) represents the percentage of instances that are actually rendered.

In order to fill histograms with the correct value, we perform book-keeping of both clipped and visible instances, which we recompute after each changes in cut objects or camera.

Histograms are sorted per compartment in a tree layout, additional histograms are also displayed for the compartments, averaging all the values of the ingredients contained inside.

Histograms are also interactive.

Upon manipulation of the right end of the second range of the histogram (light green) the system will increase or decrease the clip probability internally, resulting in changes in displayed quantities.

The culled states of the instances will get subsequently updated and counted in order to update the histogram value.

Because of the degree of indirection between the user action and the view, we are also able change the way we display information in the histograms, without affecting the way of interacting with them.

For instance, quantities are relative by default, i.e, they represent a percentage, but they can also be displayed as absolute.

For displaying absolute quantities we support logarithmic scaling to ensure low quantities to be visible in the histograms.

An logarithmic ruler is also provided to help the user understanding the displayed values

6.1. Instance Discarding

Prior to the rendering each single instance is evaluated to determine if it shall be rendered.

The cut objects how instances shall be discarded and they are applied sequentially.

Internally the filtering is applied just after the object-space culling as shown in figure XX.

First is applied the filtering based the clip probability.

For each instance, we compare a uniformly distributed random number with the clip probability.

If the random number is higher than the probability, the instance is marked as culled, and will not be rendered.

The random number is initially set for each individual instance and remain the same, in order to guaranty reproducibility of the scene.

Secondly, instances are filtered according to their biochemical properties, for each cut object and each protein types the user defines ranges values for the both quantities and molecular weight.

Instances whose properties lie outside on these ranges are marked as culled and discarded.

For the book-keeping is the clipped ingredient we count for each ingredient type how many instances where discarded in total, for all active cut object.

7. View-Dependent Clipping

While object-space culling using primitive shapes allows for a great degree of flexibility, it requires cumbersome manual operations for complex set-ups, and is also limited in terms of shapes diversities.

We additionally provide a method to specify a set of ingredient types as focus, and to selectively remove occluding instances.

7.0.1. Mask-Based Approach

Due to the potentially large number of instances in our scenes, we use accelerate the computation of occluding instances using an image-based approach on the GPU.

To determine what instances are in front of the focus, we first separately render a mask containing all the focus elements.

Focus ingredients are priorly selected from the histogram view via a dedicated toggle.

There can be only one mask created per cut object.

The mask is rendered using bounding sphere in order to lower to cost of the additional render pass.

The render pass sets the depth buffer in order to let subsequent draw calls to pass only if they are overlapping the focus region.

Subsequently, we draw the bounding sphere of the remaining instances over the mask, fragments that will pass the depth test are therefore guaranteed to belong to an object occluding the focus, with at least one pixel.

From the fragment program we then mark the occluding instance as culled, in a similar way as we would normally cull an instance.

7.1. Aperture Effect

Image-based mask culling using depth and stencil test

7.2. Aperture Effect

Image-based mask culling using depth and stencil test

8. Depth cues and Enhancements

9. Results and Discussion

10. Evaluation

11. Conclusions

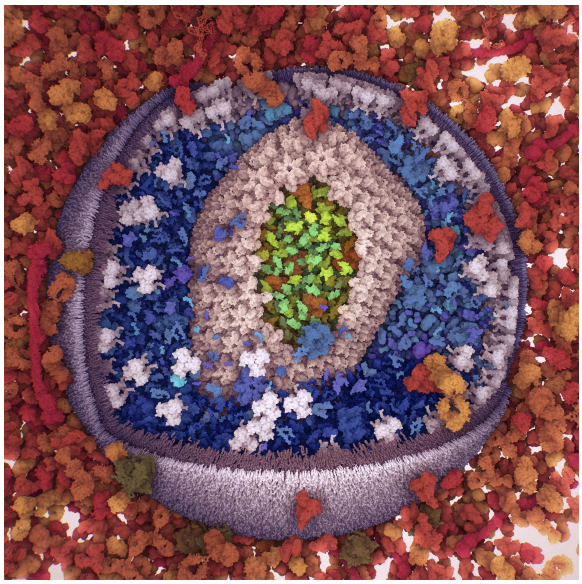

Figure 6: An illustration of the HIV virus in the blood serum utilizing cutaways created with our approach.

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