# 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 form 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 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
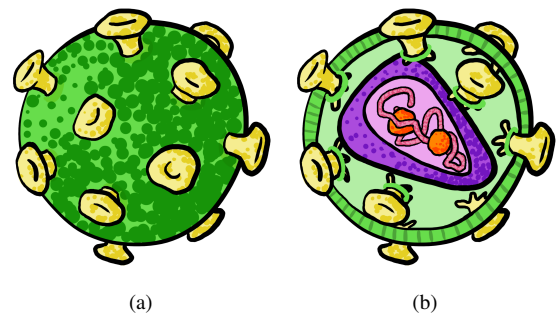


Figure 1: (a) Illustration of a HIV virus. Here, outside membrane of the virus particle is visible. (b) Cutaway view of the HIV virus. Despite the cutaway, some of the glycoproteins (yellow molecules) are kept in the view to provide adequate context.

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

### 2.1. Occlusion Management

Related occlusion management techniques can be categorized into object centric approaches and transfer function based approaches. In object centric approaches, the geometry or parts of the volume that are obstructing one or more particular objects of interest are (partially) removed. In Transfer function based approaches, the user assigns importances to intervals of the volume data values.

**Object Centered Approaches.** Cutaway and ghosting techniques were first introduced by Finer & Seligmann in 1992 as an automated approach for generating illustrations that consider the occlusion of user defined objects. In 2002, Diepstraten et al [diepstraten2002]picked up the technique again and defined a set of rules for computer-based rendering of technical illustrations to achieve a view-dependent transparency model that mimics the ghosting techniques of technical illustrations. They later extended these rules for interactive cutaway illustrations [diepstraten2003].

Analogous to the cutaways for polygonal representations, WeiÃ§kopf et al. developed an interactive clipping technique for volume rendering that supports complex clipping geometries. In 2004, Viola et al developed an automated approach for focus & context visualization for segmented volumetric objects. An assigned object importance determines the visibility priority for the segmented parts of the volume. contextual information is kept in regions where the context does not occlude the feature of interest. Follow-up work focused on the definition of levels of sparseness and importance compositing for cutaway and ghosting calculations [importance driven feature enhancement]. In 2005, Viola et al. give an overview of current âĂIJsmart visibilityâĂÏ techniques that comprise expressive visualization techniques that smartly uncover the most important features of the displayed data, such as cut-away views, ghosted views, and exploded views. baer et al published a perceptual evaluation of smart visibility techniques for two ghosted view approaches in comparison to semi-transparent approaches. the results clearly favored the ghosted view techniques. [which part of your phd thesis should I highlight?]

A. KrÃijger et al. combined visualization and interaction techniques such as cutaway views, silhouettes and color-coded distances to improve the spatial perception of feature arrangement for surgical planning. lymph nodes are emphasized using ghosted views to easily convey their spatial position. J. KrÃijger developed a system that applies transparency and shading to enable focus&context visualization in volume data sets with a simple point&click interface.

li et al developed an approach that allows interactive exploration of complex models, e.g., mechanical or anatomical, that requires the user to rig each part of the respective model. Based on the rigging, the system produces cuts that adhere to a set of rules that were inspired by anatomic

and mechanical illustrations. the approach by burns & finkelstein for view dependent cutaways inspired our aperture that is discussed in section Y. the cutaway shape is determined by the enlarged shape of the focus objects in the depth image. to preserve the information of the cut geometry, they apply shading & contouring/outlining of the cut surfaces, and ghosting of the cut geometry contours. lawonn et al extend this approach to present a composite technique that combines the visualization of blood flow with the surrounding vessel structures. the structures visually encode the wall thickness as colored regions in order to preserve important context information. a view dependent peel-away approach for volume data was proposed by Birkeland and Viola. the approach by Diaz et al preserves the relevant context information in volume clipping by allowing the user to extrude segmented surfaces such as bone structures from the clipping plane.

Sigg et al propose an approach for automatic cutaway box placement with optimized visibility for target features that are specified as degree-of-interest functions during interactive visual analysis of the volume data. Lidal et al. defined design principles for Cutaway Visualization of Geological Models. they promote boxes as ideal cutaway shapes for emphasizing the shape and depth of focus features in layered structures, such as geological sediments. illumination should effectively communicate the shape and spatial ordering inside the cutaway, as well as enhancing relationships between the focus features and the context. they define five design principles that we discuss in section X in relation to our approach.

**Transfer Function Based Approaches.** The context-preserving volume rendering model proposed by Bruckner et al is an extension of direct volume rendering. The technique uses a function of shading intensity, gradient magnitude, distance to the eye point, and previously accumulated opacity to selectively reduce the opacity in less important data regions. Contours of surfaces that would be removed due to opacity remain visible as the amount of illumination received is taken as a measure whether a point should be visible or not. Burns et al propose a multimodal approach that combines CT scan data and realtime ultrasound data. Importance driven shading is used to emphasize features of higher importance that have been revealed through the culling/ghosting.

The notion of visibility histograms proposed by Correa et al. inspired our visibility equalizer metaphor. These histograms represent the distribution of visibility in a volume-rendered image and should help users manage a set of transfer function parameters to maximize the visibility of interesting intervals in the volume.

Ruiz et al. propose an approach for automatic transfer function optimization. The transfer functions are obtained by minimizing the informational divergence or Kullback-Leibler distance between a user specified target distribution

and the visibility distribution captured from certain viewpoints.

[conclusion of the occlusion sub-section] Transfer function based approaches are well suited for volumetric data that contains segmentable structures, such as the organs or bones in a medical scan. For molecular data this only holds partially true, as some types of molecules do indeed form solid structures that could be made visible with a TF (membranes, nucleus). On the other side, within these structures there is a more noise like distribution of these molecules that cannot be segmented into solid structures. In regard to object centered approaches, (partial) occlusion of individual molecules is not an issues as the data does not contain large singular entities such as polygonal or segmented volumetric objects where each single one has a semantic meaning. instead there are thousands or hundreds of thousands of instances that belong to a couple of dozen molecule types. our approach is therefore fundamentally different from existing occlusion management approaches as it combines principles from object centered and transfer function approaches.

### 2.2. Visualization of Molecular Structures

The visualization of the molecular structures in our approach is based on the publicly available cellView [le Muzic et al.2015]. The tool is capable of rendering structures that are comprised of several billions atoms at interactive frame rates in multiple levels of detail. Lindow et al. [LBH12] were the iňĄrst to introduce a fast method for the real-time rendering of large-scale atomic data on consumer grade hardware. Similar to cellView, they utilize instancing on the GPU to repeat these structures in the scene. For each molecule type, a 3D grid of the atoms is created and stored on the GPU. Falk et al. [FKE13] further refined the method with improved depth culling and hierarchical ray casting to achieve faster rendering performance for even larger scenes.

In the domain of dedicated large scale molecular visualization, our approach is the first to introduce illustrative occlusion management techniques.

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

## 3. Overview

- We conceptualize the cutaway authoring as two stage process, as mentioned in the intro
- We use cellView
- In the first step, we want arbitrary culling shapes, so we use distance fields
- Molecules before and after cutting test are counted in the first step, so that histograms can be shown
- In the second step, we need to change the visibility, so we make the culling objects fuzzy - some removed molecules are reintroduced, some non-cutaway molecules are removed. This has to correspond with the histograms, so that this could be set by dragging histograms.
- We also introduce decay curve, so that the fuzziness doesn't have to be uniform, but it can change according to the distance from the cutting surface - we can do this since we sue distance fields for cutting.
- We also do shading of the cutaway parts so that the cut shapes are easily perceivable.

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

## 4. Workflow

Cull objects are defined...

## 5. Property-Based Clipping

Our data comprise of a dense set of macromolecules, encapsulated in compartments with several degrees of nesting.

Molecules are grouped by type and compartment, this information is contained in the scene file generated by cellPACK.

Basic filtering parameters allows to manipulate the visibility of entire set of instances based on their type, independently or not from a geometrical cull object.

Each cull object has its own parameters which are defined for all the ingredients type as shown in the overview figure XX.

When a geometrical shape is associated to the cull object, the filtered visibility will only be applied to the region defined by the geometry, e.g, plane, sphere, cone...

User can modify these filtering parameters via the user interface.

There are two parameters that are not directly related to object-space or view-space cull geometries.

First is the percentage of visible elements of a given type. We refer to this value as ingredient clip probability.

Second are the biochemical properties such as mass or quantities.

Additionally, there are more parameters which can influence when an instance is culled and which are depending on an actual geometry cull object, those are defined in section XX.

### 5.1. 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.

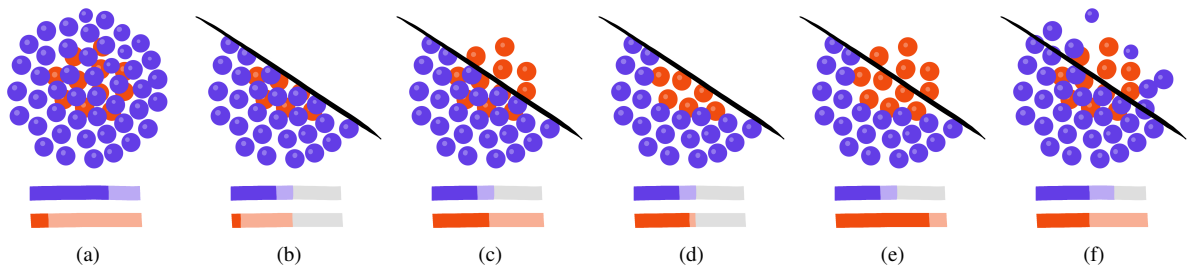Because of the degree of indirection between the user

Figure 2: Visibility Equalizers.

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

### 5.2. 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.

## 6. Shape-Based Clipping

### 6.1. Object-Space

The basic parameters of the cull objects define the global number of clipped instances for each ingredient type.

Additionally, they can be associated with geometrical shapes to determine where the clipping should take place.

#### 6.1.1. Analytical Distance Evaluation

At the very beginning of the process, for each instance, prior to the filtering, we determine if the instance if located in the region defined by the geometry.

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

Although simple, it may still be computationally expensive to evaluate the signed distance of those shapes with a large number of points in space, using a mesh-based representation.

To accelerate the computation we solve the problem analytically using a signed distance field (SDF).

Using such analytical representation reduces the problem of evaluating the distance to solving trivial 3D shapes equations.

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

The effect of the shape-based clipping can also be inverted by inverting the result of the signed distance function, offering more usage flexibility.

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

#### 6.1.2. Gradient Clipping

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

## 6.2. View-Space

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.

### 6.2.1. 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.

### 6.2.2. Aperture Effect

Image-based mask culling using depth and stencil test

## 7. Depth cues and Enhancements

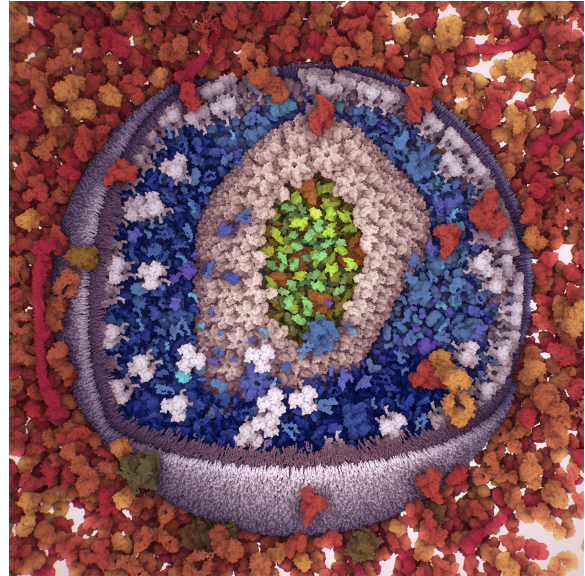## 8. Results and Discussion

## 9. Evaluation

## 10. Conclusions



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

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