A Multi-Scale Animation Framework for Biological Fibrous Structures

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Abstract

Fibrous structures are ubiquitous in cell biology and play essential structural and functional roles in the life cycle of a cell. They are long polymers, such as DNA carrying genetic information, or filaments forming the cytoskeleton, crucial for cell division and maintaining the cell shape. In order to disseminate new findings of such structures to peers or a general audience, animated 3D models of these structures have to be created, as they are too small to be imaged with microscopes. However, this is a tedious task carried out by scientific animators, who manually create expressive visual representations of biological phenomena. In this work, we present a novel concept which simplifies the process of animating multi-scale procedural models of biological fibrous structures. In contrast with existing work in the domain of molecular visualization, our approach can also capture dynamics, which are important to show when communicating biological processes.

CCS Concepts

- Computing methodologies → Procedural animation;

1. Introduction

The dynamics of molecular biology including fibrous structures are subject of intense study. Visualization of such dynamics reveals their motion, and shows the underlying mechanics of the tiny machines that are essential for every living being. Biologists often display their findings about the nanoscopic structures by the means of illustrations or animations. This is a time-consuming and expensive task typically carried out by scientific animators who carefully study underlying biology data and their functioning. Every time the data or the knowledge about the structure changes, the animation has to be remade.

Procedural Animation offer a solution to this issue by automatically generating animations for diverse input parameters. This is a well known concept in computer graphics and visualization and regularly used to generate for instance clothing [RPC\textsuperscript{10}] or clouds [SSEH03]. However, existing approaches do not address the specifics of multi-scale models consisting of many instances, such as molecular scenes. We present a novel approach for designing procedural animations in multi-scale environments.

2. Multi-Scale Procedural Animations

We divide the generation of procedural animation of fibrous structures into three parts, the backbone generation, the detail insertion and the generation of the animation.
2.1. Backbone Generation

First, we generate the backbone of the fiber, which is represented as a spatial curves on the cellular scale. We utilize a random walk to generate the backbone, which originates from a point inside of the cell and iterates until a stop criterion is reached. A random walk is a stochastic process and often used to model various real-world phenomena, such as movement or growth. A random walk consists of successive steps, whereas the direction of each step is chosen randomly. To incorporate a certain stiffness into the model, the direction is constrained and depends on the direction of the previous random walk step. In molecular scenes, the fiber structure is typically located inside of compartments such as cells or viruses. To generate microtubules inside a cell, we use a segmented 3D volume of a human stem cell, scanned with fluorescence microscopy, as shown in Figure 2 (a). The result of the random walk provides the backbone of the fiber, depicted in Figure 2 (b).

2.2. Detail Insertion

In the next step, shown in Figure 1 (a, c), the backbone is replaced with the actual structure using molecules in atomistic detail taken from the Protein Data Bank [BWF00]. The detail is generated according to a certain procedure, which is dependent on the structure. For instance, microtubules are generated by creating rings around the point of the backbone curve, as shown in Figure 2 (c). The building blocks of the microtubules are aligned with the tangent of the curve in the given point. For each point a certain number of building blocks are inserted, each with a specific offset.

This process is applicable for various fibers architectures, e.g., also for DNA structures [HLLF13]. Figure 2 (d) depicts a standard model of the B-DNA double helix consisting of individual base pairs with an angular offset of 34.3° and a spacing of 3.4Å between each base. To apply the angular offset we rotate the normals of the curve accordingly and inject a DNA base pair for each point.

2.3. Procedural Animation

In the third step, shown in Figure 1 (b, d), various properties are calculated to create complex animations of the generated fibers. An example of such animations is the biological process of assembly or disassembly of a polymer structure. However, we can also create animations which do not replicate naturally occurring processes, but they are purely illustrative. One example of such a illustration is the continuous unwinding of a DNA helix to reveal the atomic structure of the individual base pairs.

For this purpose, we develop a shader-based framework, which can be included in the existing visualizations. The framework processes the fibers generated in the previous steps and exposes information to the programmer that can be used to create multi-scale animations. On the largest (fiber) scale, this information includes position along the fiber, tangent and normal vector, and the segment currently undergoing the given transformation. On the molecular scale it is the sequence number of individual molecules along the fiber, and optional clustering information (such as affinity to a certain sub-filament, such as individual strand of a DNA). On the atomic scale, it is a unique atom ID, molecular chain ID, etc. With this information, the animations of various transformations that the fibers undergo can be created. An example can be seen in Figure 3, where a transformation was applied to a model of a DNA molecule, where a part of the double helix is unwound to reveal the internal atomic structure of the molecule. The framework enables the users to create continuous animated transitions between the individual states, where the transitions are governed by specified molecule paths. In this way, the transitions illustrate various dynamic biological processes, but also artificial illustrative animations.

3. Conclusions

We have discussed a novel concept of approaching animation of dynamic processes in multi-scale, multi-instance molecular scenes. We believe the concept to be useful for the visualization of various naturally occurring dynamic processes.

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References


