Spatially Continuous Change of Abstraction in Molecular Visualization

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Abstract

Based on an approach for the temporal change of abstraction in molecular visualization we describe how to achieve a spatially explicit control of abstraction. This allows us to depict different abstraction stages of a single molecule in a single still-image visualization. This approach works best for long, linear molecules with repeating substructures that allow viewers to visually compare the continuous representational changes of these parts.

Index Terms: I.3.m [Computer Graphics]: Miscellaneous—Scientific Illustrative Visualization, Molecular Visualization

1 Introduction and Motivation

Abstraction plays an essential role in molecular visualization because the important bio-chemical processes occur at different levels of scale of the involved biological structures. Traditionally, both illustrators and software tools have employed/provided a number of well-defined abstraction types including the space-fill diagram, the balls-and-sticks model, the licorice visualization for the primary structural depiction, and backbone and the ribbon model for communicating the secondary structural arrangement within the macromolecule. While these abstraction communicate internal structure of a molecule, tertiary and quaternary structure describe the outer appearance of the molecule. All corresponding abstraction stages, however, are distinct forms of depiction that are separate from each other and whose (spatial) relations with each other are not always easy to understand. In a recent paper [1] we demonstrated how to emphasize this spatial connection between some of the internal abstraction types by facilitating a seamless transition between the space-fill, balls-and-sticks, licorice, backbone, and ribbons abstraction stages. Moreover, we integrated this one axis of abstraction into a *three-dimensional abstraction space* that also allows us to explore molecular abstraction with respect to the 'illustrativeness' of the depiction and the support of spatial perception.

Nevertheless, this interactive exploration of the different forms of abstraction in molecular visualization [1], at any given time, only provides visualizations that represent a single point in the abstraction space. Consequently, the use of interaction is essential to the approach to be able to transition over time between different stages in order to understand the relationships between them. However, in some cases it may be beneficial to be able to visualize *different abstraction stages* of a single molecule in a *single visualization* to be able to understand them without the need for animation or interaction. In this case the transition of abstraction would not happen temporally but *spatially*, for example along the backbone of a longer molecular structure. Molecules with repeating structures such as DNA or RNA, and certain proteins are particularly well suited for such an approach because the viewer can understand the representational changes introduced by the different levels of abstraction by comparing the depiction of the several repeating substructures of the molecule. In this way our new approach with *spatially continuous abstraction* facilitates an integrated visual communication of the multi-level molecular structure and, thus, provides a more complete visual description of a molecule's structural and, potentially, functional characteristics.

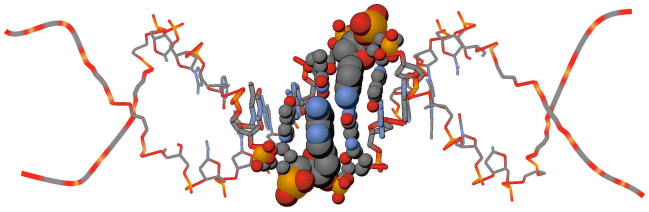

Figure 1: DNA illustrating the spatial control of abstraction.

Seamless spatial transition between visual abstractions is well-aligned with the principles utilized in the craft of molecular illustration. Illustrators are taking the advantage of perceptual and cognitive capabilities of the viewer, in this case the *object constancy*, so that multiple aspects of the molecular structure are simultaneously communicated through the resulting illustration. We adapt this illustration concept for interactive data visualization.

2 Realization

A spatially continuous structural or illustrativeness abstraction at a single point in time requires, for each atom or bond, a parameter t_s and t_i such that we can determine the abstraction $f(t_s)$ and $f(t_i)$ for the entire molecule (following van der Zwan et al.'s [1] notation). We determine these parameters by first identifying the molecule's backbone and then using it to define the change of structural or illustrativeness abstraction along its length. Next, we propagate these parameters to the rest of the molecule by simply assigning the specific values of t_s and/or t_i, at locations where a non-backbone structure connects to the backbone, to the entire non-backbone structure.

These parameters are passed to the shaders that determine the rendering of the structurally abstracted molecule as well as its illustrativeness. Even though the the parameters are only defined once per atom/bond or once per amino acid, the relatively small size of these elements when compared to the entire molecule results in viewers perceiving a gradual change of the two types of abstraction (Fig. 1). Moreover, we do not change the abstraction by means of support of spatial perception in this spatially explitit manner because of the global nature of perception—we believe that different forms of support of spatial perception in a single image would confuse viewers.

3 Results and Discussion

Fig. 1 shows the general approach: instead of applying the same level of structural abstraction to the whole DNA molecule as in [1], we use a higher structural abstraction level overall and apply less abstraction only to a localized part of the two strands (Fig. 1, bottom) to show that part in detail. This continuous change of abstraction can easily be understood by viewers due to the DNA's repetitive structure and further illustrates the fact that only a small segment is being shown. To illustrate the application for a less regular molecule, Fig. 2 shows an example where the spatial control of structural abstraction has been applied to different regions

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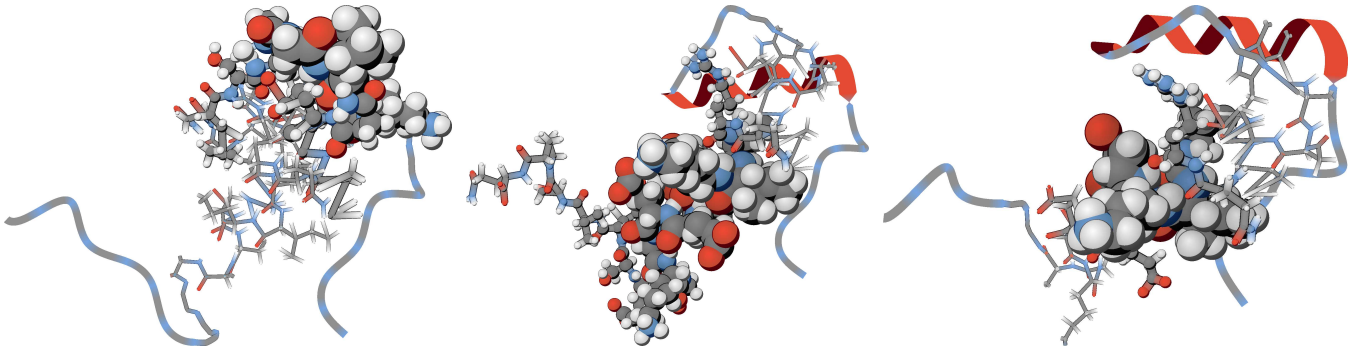

Figure 2: Proteins with structural abstraction applied in a localized fashion.

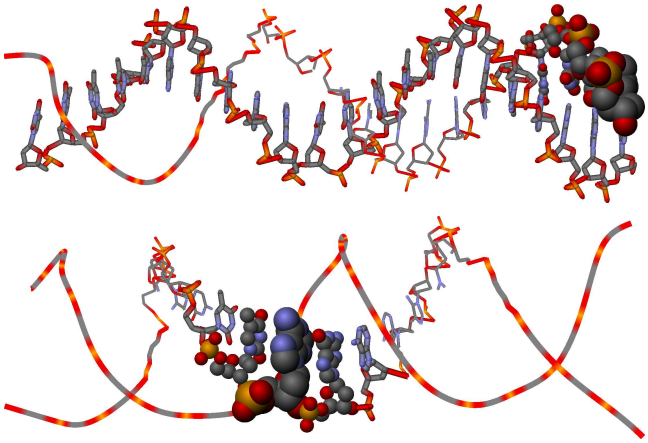

Figure 3: DNA and selective structural abstraction.

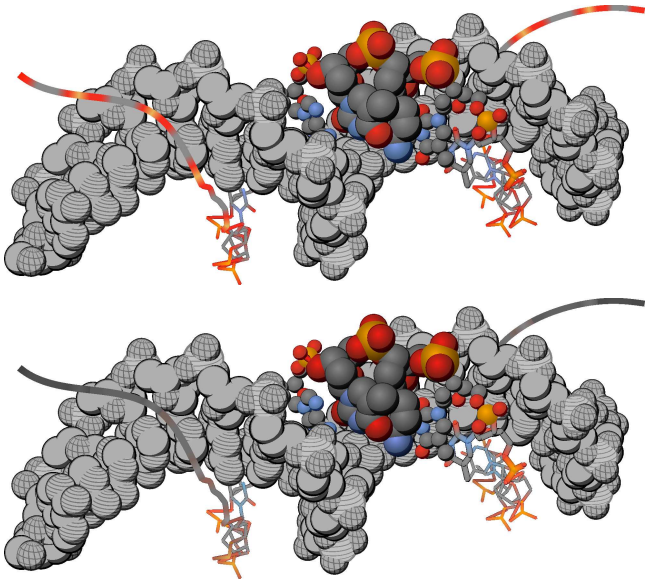

Figure 4: Structural abstraction combined with abstraction by means of illustrativeness.

on the backbone of the same protein, using varying parameterizations. This facilitates the highlighting of certain regions on a large molecule while less essential ones are shown in a structurally abstracted way. Fig. 3 shows more examples of selective structural abstraction, in this case (as opposed to Fig. 1) only applied to one strand of a DNA section. However, by also using selective abstraction of the illustrativeness axis as shown in Fig. 4 we can further emphasize certain aspects of the molecule such as one strand of a DNA section. Here, simply the application of a constant (high) illustrativeness to the part of the DNA that is not in focus places emphasis on the other strand (Fig. 4, top). If we now control the illustrativeness of the strand of the DNA that is in focus similar to how we control its structural abstraction (Fig. 4, bottom) we can further concentrate the focus to the one single part shown in detail. Finally, Fig. 5 illustrates the interaction between two molecules, with the specific interaction site emphasized in low structural abstraction.

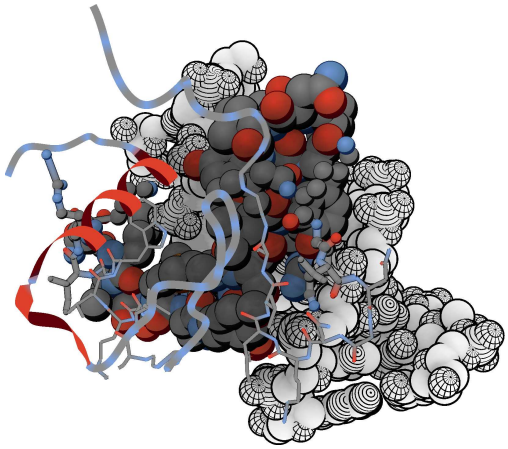

Figure 5: Interaction of a protein with another molecule.

4 Conclusion

Seamless transition between visual abstractions is effective for communicating how different structural aspects relate to each other. This transition can be realized over time in an animation or spatially, e. g., along the strand(s) of the macromolecule. Further work to strengthen the communication of the hierarchical aspect of the structural arrangement in proteins, for example, can be oriented on the role of graphically embedding of one visual abstraction in its hierarchical parents.

References

[1] M. van der Zwan, W. Lueks, H. Bekker, and T. Isenberg. Illustrative Molecular Visualization with Continuous Abstraction. *Computer Graphics Forum*, 30(3):683–690, May 2011. doi> 10.1111/j.1467-8659.2011.01917.x