Tangible Augmented Interfaces for Structural Molecular Biology.

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1. Introduction.

The evolving technology of computer auto-fabrication ("3-D printing") now makes it possible to produce physical models for complex biological molecules and assemblies. We report on an application that demonstrates the use of auto-fabricated tangible models and augmented reality for research and education in molecular biology, and for enhancing the scientific environment for collaboration and exploration. We have adapted an augmented reality system to allows virtual 3-D representations (generated by the Python Molecular Viewer) to be overlaid onto a tangible molecular model. Users can easily change the overlaid information, switching between different representations of the molecule, displays of molecular properties such as electrostatics, or dynamic information. The physical model provides a powerful, intuitive interface for manipulating the computer models, streamlining the interface between human intent, the physical model, and the computational activity.

Computer-generated physical models allow direct experience of the complex shapes and relationships of biological molecules (Bailey 1998). Coupling these models with computational input and output provides a natural interface between the user and the wealth of data coming from the structural biology community. Physical molecular models, while vastly more informative and intuitive than 2D drawings or textual descriptions, are fixed in form and are limited in the number of properties they can represent. We use computer-based spatial tracking and rendering methods to enhance the semantic content of our models and to show dynamic properties.

2. System.

We have developed a software framework to enable the fabrication design and augmented display of the models to be performed within the same environment. The physical models can be specified by a wide range of molecular computational models, including molecular surfaces, extruded volumes, backbone ribbons, and atomic ball and stick representations. Our development is based on the extensible Python Molecular Viewing environment (PMV) (Sanner 1999), a modular approach to molecular modeling. PMV is built within the interpreted language Python.

Our AR interface combines real-world presence with virtual object presence. The user manipulates a model and the model is tracked by a video camera and displayed on the computer screen or in a lightweight head mounted display. A virtual model (e.g., another 3D rendering of the same model, textual labels, or a 3D animation. An electrostatic field is shown on the virtual model in the figure 1) is superimposed over the video image, and spatially registered with the model as the user explores the structure. The result is a quite compelling sense of virtual object realism. Our approach is based on the widely used ARToolKit. By using several markers, the AR overlay can be maintained and appropriately occluded (figure3) while being arbitrarily manipulated. We will demonstrate how the interface is use to steer molecular computation. The interface allows getting quantitative interaction energy as tangible models are manipulated.

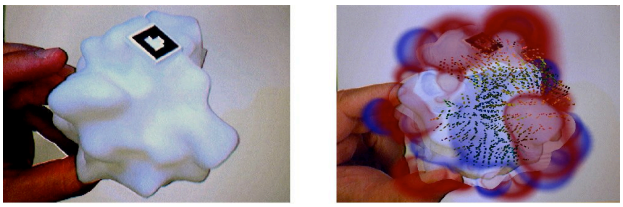

Figure 1: model of superoxide dismutase built with the Stratasys machine Prodigy Plus(left), overlay showing a volume render electrostatic field and animated electrostatic field vectors (right)

3. Future Work

We will develop a spatially tracked “data probe’ designed to enable interaction with both physical and virtual models. Our system currently relies on fiducial tracking markers, we will develop new algorithms and code for markerless spatial tracking of our models which will be added to our system. We will explore the use of new visualization techniques to facilitate query operations in the context of this unique interactive environment.

4. References

Bailey, M., Schulten, K. and Johnson, J. (1998). "The use of solid physical models for the study of macromolecular assembly." Curr Opin Struct Biol 8: 202-208.

Sanner, M. F. (1999). "Python: a programming language for software integration and development." J Mol Graph Model 17(1): 57-61.

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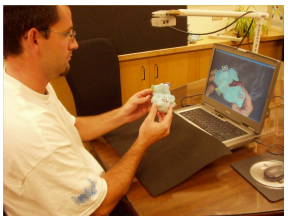

Figure 2:
A user is holding a tangible model of 30S Ribosome subunit, the computer screen displays AR added 50S ribosome subunit which assembles with the 30S.

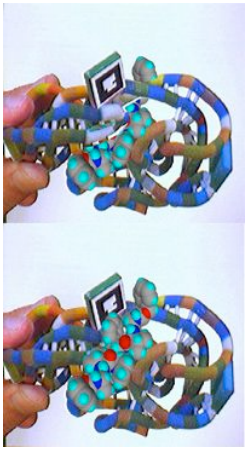

Figure 3:
Physical protein backbone representation of HIV protease with computer graphic display of tl3 inhibitor. The pictures show the use of masking to give a compelling sense of virtual object realism. The top picture shows the scene with the mask using the geometry of the tangible model as the mask. The bottom picture shows the composite image when the masking is not in use. Notice how the three red oxygen atoms appear to be under the protein chain in the top image, while in the unmasked image the virtual component appears in front of the physical model.