Interactive Molecular Visualization

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Using a model description in order to arrive at a deeper level of insight and a higher level of understanding is at the heart of our scientific culture. With regard to chemical and biological structures, molecular visualization serves as an interface in the process of assembling information to construct a model, and is of assistance in validating and analyzing the obtained model to arrive at a functional explanation. As only a limited portion of these procedures can be automated, and because the process of verification and refinement requires constant feedback from the scientist, interactive control is essential to the sucess of model building and analysis.

The wealth of information that forms the basis for structural models comes from a variety of sources that are both of experimental and theoretical origin. Methods such as X–ray crystallography, NMR spectroscopy, electron microscopy, scanning probe microscopy and computational chemistry all produce structural information, but each method has its own characterisitcs, strengths and weaknesses. The integration of all pieces of the puzzle to produce a coherent and conclusive picture is in itself a significant challenge.

Over the last few years, a variety of novel techniques for interactive molecular visualization have been invented. Fast surface generation, property mapping, information filtering and real–time volume rendering provide the scientist with an arsenal of visualization tools more powerful than ever. The track on "Interactive Molecular Visualization" is intended to provide a forum for highlighting and discussing the latest concepts and techniques related to interactive model construction and analysis using computer graphics.

In the following papers, a variety of aspects pertaining to the visualization of molecular information are presented. Shimura *et al.* explain how state–of–the–art modeling techniques can be employed to solve a biostructural problem. Gernert *et al.* move on to a more logical breakdown of molecular structure, whereas Edelsbrunner *et al.* formalize concepts of molecular surface geometry. Johnson and Zsoldos introduce a complete modeling package that integrates mechanisms to investigate molecular interaction. The last two papers present molecular visualization in the context of communicating structural information: Vollhardt and Brickmann concentrate on the transfer of visual structural information, while Ihlenfeldt and Gasteiger include other sources of molecular data, both using the world–wide web as a communication gateway.