Computer graphics has evolved into the principal modeling tool in biomolecular structural studies. It is used extensively in molecular modeling building, evaluation, and presentation. Hardware and software now exist that enable these activities over a wide range of cost and performance, from personal computers to supercomputer class devices. This paper will review the current application of computer graphics to biomolecular modeling, focusing on the special requirements of each of the principal modeling functions: synthesis, analysis, and communication. Emphasis will be given to developing technologies and high-end performance.

In the hardware arena, new classes of machines have recently appeared that will have significant impact on molecular graphics. The evolutionary growth of the scientific workstation is now at the stage where machines with near supercomputer power and integrated high performance graphics will soon become available. Workstations from Data Corporation and Stellar are of this class. A new class of machine, the application accelerator will produce similar performance by attaching to existing workstations. The recently announced TACC-I from Transcept Computer is an example of this type of hardware. Special purpose graphics engines using highly parallel computation are currently prototyped to out-perform all existing display systems. The Pixel Play machine from the University of North Carolina, will be discussed as an example of this trend.

Software seems to be the major bottleneck in current molecular graphics. We are in a period of transition from home-built systems to team-built commercial systems. The problem in the near term will be the flexible incorporation of new algorithms from the molecular modeling community into a widely distributed package. Discussion will also touch upon the status of graphics standards and new tools for constructing user interfaces.

The application of computer graphics problems in biomolecular structure will be illustrated by work from the author’s laboratory. An example of synthesis activity will be given by discussing the modeling of a novel DNA intercalation mechanism. Analysis activity will be illustrated with the examination of protein-protein interactions from home-built systems to team-built commercial systems. Finally, special purpose graphics engines using highly parallel computation are currently prototyped to out-perform all existing display systems. The Pixel Play machine from the University of North Carolina, will be discussed as an example of this trend.

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