highly irregular surfaces, but where certain surfaces features endow the molecule with the property of specifically recognizing and binding to other molecules. In the case of globular proteins, these recognition phenomena include the binding of specific ligands that may alter the properties of the protein or of the ligand itself, and the association of the protein with other proteins, with sugars, nucleic acids, or lipids. In order to understand these phenomena fully, a complete audit of the various energetic contributions to the interaction is required, but it cannot have escaped the notice of anyone studying these processes that the shape of the complementary binding regions of two molecules participating in the binding is an important feature. The natural explanation for this is that the shape of a region on the surface implies a specific spatial distribution of the atoms, electrons, etc., which are responsible for the energetic contributions to the interaction, be it charge, van der Waals interactions, polarizabililty, and so on.

A new type of shape descriptor has been developed for use in the study of biomolecules, which is a three-dimensional (3D) version of a Fourier shape descriptor technique already developed for pattern recognition of 2D objects, such as machine parts and radar images of aircraft. The 3D version, which employs spherical harmonics, has been used to describe the surfaces of globular proteins[3] and the contact interfaces of protein-protein and enzyme-substrate complexes.[4] The coefficients obtained in the expansion in spherical harmonics represent the shape descriptors themselves, and their magnitude allows one to make a quantitative estimate of shape similarity between two shapes or between contingent surfaces on interacting molecules.

In the early stages of this work, only van der Waals surfaces have been considered, but the method is easily adaptable to the case of charge or other kinds of interaction.

Fourier methods lend themselves naturally to a consideration of spectral analysis. The methods employed here enable one to construct "shape spectra" of molecules. From such spectra for two molecules known to bind to each other, it is possible to extract the common features that correspond to their congruent surface binding regions. In this way it is even feasible to contrive routines for "automatic docking" of two molecules in cases where it is not known how they associate with one another.

1 Connolly, M. L. Solvent-accessible surfaces of proteins and nucleic acids. *Science* 1983, **221**, 709–713
2 Connolly, M. L. *J. Appl. Cryst.* 1983, **16**, 548–558
3 Leicester, S., Bywater, R. and Finney, J. L. *J. Mol. Graph.* 1988, **6**, 104
4 Leicester, S., Bywater, R., and Finney, J. L. (in preparation)

Molecular Graphics Software on a Raster Device

Josette Lamotte,† Georges Dive,† Dominique Dehareng† and Philip Staiger‡

†Université de Liège, Service de Microbiologie, Institut de Chimie, B6, B–4000 Sart Tilman (Liège), Belgium
‡Megatek Corporation, 9645 Scranton Road, San Diego, CA 92121, USA

Most recent developments in molecular graphics software attempt to drive raster device hardware. High-resolution and fast three-dimensional (3D) local transformations have been achieved in new graphics processors. At the Microbiology Lab, University of Liège, a Megatek 9300 is linked to a VAX 11/780 through an Ethernet interface.

On the same bus are connected several local processors with specific functionalities, such as real-time manipulations of 3D wire-frame and shaded objects and z–buffering with hidden-surface removal.

Through the Local Task Language, graphic objects refer to host entities that can be organized into a hierarchical database by FORTRAN-callable subroutines (APPRENTICE). Moreover, the communication protocol allows a full dialog between the application program running on the host and the graphic processor.

To begin with, two well-known programs have been adapted to the 9300:

- PAKGGRAF, from the Department of Biological Sciences of Columbia University, has extensive facilities for handling protein data sets, including connectivity changes, rigid motion of the whole molecule, or "jiggles," energy calculation and minimization. We have improved this last feature and written the visualization tools using interactive devices.
- FRODO, first written by Alwyn Jones (Wallenberg Laboratory, University of Uppsala, Sweden), is used worldwide by protein crystallographers as well as in molecular modeling applications. The graphic part of the E&S MPS (B.L. Bush, MSD and Co.) was converted into MEGATEK software, giving rise to an efficient real-time version.

At last, we have developed software for calculating and representing 3D electrostatic potential maps at the quantum chemistry level.

These graphic developments are the first step of a wider project that has to be seen as a more general program in the molecular interaction study.

Extracting Conformational Information from Molecular Dynamics Trajectories Using Digital Signal Processing Techniques

D.J. Osguthorpe
Head of Molecular Graphics, School of Chemistry, University of Bath, Bath, UK

New techniques will be presented that allow conformational information from molecular dynamics trajectories to be analyzed and displayed on interactive computer graphics systems.