tile is limited. Then a simple hidden-surface algorithm can be used on the limited data.

For example, if a van der Waals surface picture is being prepared, there might be, say, 50 atoms impinging on a given tile in projection on the screen. The specifications of the atoms are initially sorted by closeness to the viewer, and the new algorithm can then perform a very fast hidden-surface elimination for any given pixel within the tile. The algorithm starts with the atom closest to the viewer and works its way down the list until it gets to an atom that cannot possibly have a surface point closer to the viewer at the given pixel position than the closest atom yet chosen. In the language of computer graphics, this algorithm is said to use a priority list combined with z-buffering.

Once the hidden surfaces have been eliminated, and it is known which parts of the molecule are in shadow, the shading computation is straightforward and in the present case is based entirely on Chapter 16 of Foley & van Dam,[1] with specular reflections approximated using the Phong model.

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Protein Surface Analysis: Qualitative Approach Using B-spline Functions and Quantitative Comparison

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A new way to describe protein surfaces is suggested, bringing out the interesting potentially functional features to facilitate their analysis and comparison. The classical representation of molecular surfaces (often calculated with the algorithm of M.L. Connolly[1,2] is very efficient for detailed surface examination but is unsuitable for an overall view, the few significant features being buried in many small amplitude bumps. In order to improve this representation of protein surfaces, we use B-spline functions,[3] smoothing the surface iteratively from atomic details to overall shape.

The program SURSPLIN uses, as starting data, the solvent-accessible surface of M.L. Connolly and is interfaced with the general-purpose molecular modeling software MANOSK.[4,5] It could be added easily to other software.

Up to now, SURSPLIN has been employed to study and compare more than 50 macromolecules, mainly proteins. In addition to the well-recognized active sites, a small number of conical pits, about 7Å in diameter and depth, are often encountered among interesting and repetitive topological features observed on protein surfaces.

The above comparison also shows that the rugosity of protein surfaces is variable. Several proteins, such as Azurin, are particularly smooth; others, such as Ferredoxin, possess very complex and uneven surfaces.

Currently, the splined surface is displayed by three-dimensional (3D) grids with a 50% reduction of memory occupancy, in comparison with the corresponding solvent-accessible surface displayed as dots. Large macromolecule complexes, such as the icosahedral face of a virus, can therefore be handled. Using fine grids, the splined surfaces are also valuable in displaying features of small molecules.

To complement the SURSPLIN program, we have developed a program (SURSCOP) for the analysis and comparison of quantitative aspects of surfaces. SIRSCOP allows a count of the distribution in size of topological features at the surface of molecules, which is especially useful for proteins. Typical examples of results obtained with SURSPLIN and SURSCOP programs will be presented.

The programs SURSPLIN and SIRSCOP are available upon request to the authors.

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The Quantitative Measurement of Molecular Shape and of Binding Interfaces Using Molecular Shape Descriptors

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Within the field of molecular graphics, much effort has been devoted to displaying the molecular skeleton of complex biomolecules, providing an elegant demonstration of the way in which these molecules are constructed. There is, however, a need for displaying surfaces, especially if one is interested in carrying out docking or drug design studies. Here, too, some elegant methods exist; foremost among these is the method due to Connolly,[1,2] but these methods are of use primarily for display purposes and do not give any quantitative measure of shape or of differences in shape.

The molecules of interest in biological processes are characterized *inter alia* by well-defined but apparently