often require the computation of the intersections of geometric objects, such as spheres and polyhedra.

Three such methods are discussed in this presentation: (1) a hidden-line elimination algorithm for stacked planar contours, (2) a protein surface shape measurement algorithm which intersects a sphere with a polyhedron and (3) an analytical molecular volume algorithm for the union of a set of intersecting spheres (atoms). Generalizations about geometric intersection algorithms are inferred from these three examples.

6

Transparallel applications in molecular graphics

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There has been a considerable growth of interest in parallel processing by the computational chemistry community over the last couple of years. Despite this interest, almost all the practical laboratory experience so far has been confined to Intel Hypercubes. The performance of early Hypercubes has been disappointing, although later versions incorporating a vector processor at every node should lead to increased performance. Although machines like the Hypercube are inexpensive when compared with supercomputers, they are still expensive in absolute terms (c. £200 000) and offer no performance advantages over conventional array processors such as the FPS-164.

Since these early developments, an exciting new contender has appeared in the form of the Inmos transputer. The transputer is cheap (approximately £350 for the 1.5 Mflop T800-20), ubiquitous, and very easy to design into large arrays. At the time of writing, only 0.15 Mflop T414-20 integer transputers are readily available, and the only fully supported language is OCCAM, although β-releases of FORTRAN 77, C and PASCAL are available.

The most interesting question regarding the transputer is whether the manufacturers' publicity and the undeniable promise can be translated into a system suitable for large-scale molecular graphics calculations.

Our experiments with parallel energy minimization calculations indicate that the advent of the transputer is a major landmark in the history of computational chemistry. A 64 node T800-20 system fits comfortably inside a 19 × 16 × 18 in desktop rack and offers computational performance equivalent to a Cray-1S for energy minimization and other codes. Such a system can cost well under £100 000.

The authors will discuss commercially available hardware, the programming of transputer arrays for molecular-graphics calculations, and the efficiencies of alternative interconnect topologies.

7

Model building studies in supramolecular chemistry

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Supramolecular chemistry, at the frontier of organic and inorganic chemistry, biology and physics, involves intermolecular interactions and conformational processes of flexible units, leading to the recognition of 'substrates' by 'receptors'. From a theoretical point of view, this field raises challenging problems, such as the design and construction of structures suitable for complexation (e.g. with adequate cavities), energy representation and optimization, and the treatment of solvent effects on structure and selectivity.

First, we recall the limits of two basic working hypotheses used for empirical force-field calculations: transferability of fragment properties (structural and electronic features, reactivity), and the additivity of energy components. Next, different types of empirical-energy calculations in the field of macrocyclic receptors will be presented. Molecular mechanics is used for 18-crown-6 as a flexible receptor for alkali cations, and as an anchoring site for ammonium derivatives; here the graphics system is essential for building starting structures.

The graphics system brings a major contribution in the analysis of Monte Carlo simulations on 18-6 in a water cluster: not only the hydration energy, but also the structure of water around the 'solute' depend on the conformation of the solute. Such a pattern has been confirmed since by X-ray crystallography.

Visualization of dynamic structures, from molecular dynamics simulations and normal modes of vibration, is also illuminating. Particularly, low frequency modes of vibration for cryptands and cryptates lead to the opening of the cavity. A similar process has been found recently for the active site of several enzymes. It thus provides a pathway for substrate inclusion.

There is no way of predicting computationally whether or not a substrate will bind to a receptor in solution. However, a new technique, involving stepwise perturbations from one system to another, may give relative free energies of binding.

8

Microcomputer graphics in biochemical education

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It is virtually impossible to study any biological subject at the undergraduate level without coming into contact with biochemistry at some stage. Biochemistry classes therefore tend to be large and contain students with very different backgrounds. Many students chose biological subjects simply 'to get away from maths' and these students often find such subject areas as enzyme kinetics difficult to grasp.

Other problems are posed by trying to teach a rapidly evolving subject at a time of dwindling resources. In particular, many modern techniques in biochemistry are too time-consuming, too expensive, too dangerous or simply impractical to actually carry out in the teaching laboratory.

For these reasons, we are developing simulation programs that are being integrated into the courseware. These programs rely heavily on graphics for their effectiveness. For example, in teaching enzyme kinetics, animated displays show enzyme substrate, product and