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Representation of energetic and electronic properties in enzymatic reaction pathways

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The computer system recently installed at the Microbiology laboratory in the University of Liège (Belgium) combines two host computers. A raster graphic device is linked to a Data General MV 4000 (0.6 Mips) coupled with an FPS 5205 array processor (38-bit; 12 Mflop). The FPS 164 (64-bit; 11 Mflop) is connected to a VAX 11/780. A second graphic system will be configured in the near future. Unix subset runs on both machines. The molecular applications developed by the authors attempt to study the interactions of antibiotics with the active site of D-alanyl-D-alanine peptidases and β-lactamases. Force field calculations are often used to calculate the energetic properties of molecular complexes. This approach has been successful in the determination of Michaelis complexes and tetrahedral adducts in serine peptidases. The continuous increase of the 32-bit computer power enables so called real time energetic calculations on an interactive graphic device. But, the calculations become more time consuming as the accuracy of the function terms increases. To boost this step, the 38 bit array processor FPS 5205 has been connected on the 4 Mbyte/s BMC bus of the Data General. This processor decreases the computational time of the rate limiting step and near real time applications can be run. This solution is not consistent with a delocalized graphic workstation since the graphic system has to be considered as a terminal for the host computer. Another attractive feature of an array processor in molecular graphics applications is the direct driving of the graphic memory of a raster device through an IOP. To describe electronic properties and determine the energetic and geometric features of critical points such as transition state structures, the quantum chemistry wave function has to be calculated. Depending on the extension of the basis set, *ab initio* calculations can be carried out for molecules involving 30–50 atoms. More than 50 CPU hours on a 1.0 Mip machine is required to achieve this goal for such a molecular system. From density matrix elements, mono and bielectronic properties can be calculated. The most popular one is the electrostatic potential maps of which quality is closely related to the accuracy of the wave function. All this computational effort will be hardly reduced with the 64 bit FPS 164. Two types of graphic applications will be presented. The first one is a comparison of 3D electrostatic potential maps calculated at the quantum chemistry level. The second application shows data reduction results of an energy hypersurface defined by 42 degrees of freedom. This approach is an attempt to visualize how a molecular system moves from reactants to products via the transition state on a multidimensional surface.

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'Wirrwarr': an interactive colour vector display for crystallographic applications

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An interactive line-drawing display system was designed for a beam-penetration tube (Model MD89, Ferranti) capable of representing images composed of four different colours (red, orange, yellow, green) at four brightness levels. The vectors to be displayed (maximum: 65000) are transferred via a simple 16 bit interface from the host computer to the dedicated refresh memory of the display controller. For typical applications the displayable vector length is 100 metre at 50 Hz, and multiples thereof at 50/2, 50/3... Hz refresh frequency. Using a microprocessor controlled trackerball the picture can be rotated in real time around two axes lying in the plane of the screen, one vertically and the other horizontally. The rotation is implemented by an analogue multiplication of the refreshed vector with the actual rotation matrix, the new z-coordinate being used for depth cueing. The maximum rotation speed is 180°/s. Other graphical input devices consist of a x/y-tablet and 9 potentiometers. A stereoscopic effect is generated by analogue x-shift of the perspective vanishing point corresponding to the eye separation. These shifts are synchronized with shutters rotating in front of the eyes. The design of the graphics software package was guided by the aspects of speed, simplicity and flexibility. To free the user of any address calculation within the refresh memory and to solve the colour sorting problem a simple page structuring technique has been implemented. The user conceives an image as a set of logical entities, called items. An item consists of the graphical elements point and vector. The colour of an item is determined by its identifying number. At any time graphical elements can either be appended to an item (which is initially empty) or replace an existing element. To display text, the full ASCII character set has been implemented by software. In addition individual items can be made visible, invisible or deleted. The instrument has been used so far for visualizing protein structures, electron density maps, and docking experiments of the actin filament and tobacco mosaic virus.