ELSEVIER

Personal computer–based visualization of three-dimensional scalar and vector fields: An application to molecular graphics

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A desktop PC-based graphics package, UNIVIS, for visualization of three-dimensional numerical data is described. Apart from routine molecular model visualization, the package provides for a host of other features such as extraction of various surfaces, planar cross-sections of the three-dimensional data, and property texturing. Fast rendering and transparency are the strengths of the present package. These features are comprehensively discussed. The salient features of UNIVIS are presented in the form of visualization of a variety of molecular properties, which are of immense importance in understanding molecular structure and reactivity patterns.

Keywords: molecular graphics, personal computer, isosurfaces, gradient paths, transparency

INTRODUCTION

An accurate quantum chemical description of molecular structure and reactivities has now become possible with the advent of high-speed computing. With this development, visualization has become an important tool in chemical predictions. To a practicing chemist, it is more valuable to obtain a three-dimensional representation of the molecular structure and property under consideration, rather than to read and try to interpret "numbers gushing from a computer."[1] Furthermore, visual representation of various molecular simulations and potential energy surfaces of interacting species, etc., offers better insights to the progress and pathways of a chemical reaction. For such interpretative purposes, the visual information sought out should be available as speedily as possible. Thus, emphasis should be on "visualization as research tool" rather than on "visualization as communication aid."

There are packages available for workstation environments that cater to some of the above-mentioned needs. For example, the SPARTAN[2] software provides an excellent facility for display of molecular structure, electron density surfaces, and two-dimensional slices as well as HOMO and LUMO representations and animation of vibrational modes. There are, of course, a host of other packages such as HyperChem,[3] CAChe,[4] Chem3D Plus,[5] PCModel,[6] and Molecular Editor[7] that provide visualization of molecular models. In most of the above-mentioned packages, graphics comes along with ab initio and/or semiempirical level chemical calculations. Most of the above-mentioned packages are, however, available on workstation platform alone. Yet another package, MoG,[8] available on the Commodore Amiga computer, was primarily developed for molecular structure visualization. Covic and Sando[9] have interfaced VoxelView/PLUS[10] with GAUSSIAN 85.[11] It makes use of volume-rendering techniques[12] for display of electron densities. There are ray-tracing programs available for PC-based machines such as POVRAY[13] and that developed by Kim et al.[14] These programs restrict themselves primarily to viewing of molecular structures.

From this discussion, it seems that the emphasis is on the development of visualization aids for workstations, rather than for PC platforms. Keeping in view the low cost and omnipresence of PC platform, UNIVIS, a PC-based scientific visualization software for scalar and vector data over two- and three-dimensional grids, has been developed. This article documents the capabilities of the package.

Color Plates for this article are on pages 25–27.

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HARDWARE AND OPERATING SYSTEM REQUIREMENTS

The package described in the following sections is available on IBM or compatible computers with DOS. UNIVIS is executable on 80486 CPU-based systems with an SVGA color monitor. It requires at least 2MB of memory and 1MB of video RAM (available on the graphics display card). Using 1MB graphics display memory, the program works with 1024 × 768 pixels and 256 colors. The size of the actual color image is 768 × 768, the rest of the space being taken up by menus.

PROGRAM

The present visualization program is written entirely in Fortran without use of any graphics library except, of course, the rudimentary pixel plot utility. The rationale behind such an effort is to decrease the future efforts involved in interfacing the code with other chemistry softwares (the majority of which are written in Fortran). Currently, the program accepts stored data and allows its visualization in every conceivable way. It thus operates in an off-line fashion. In future, it may be coupled with the property evaluation routines, in order to obtain virtual reality (of course, for this one needs really high-speed PCs!).

INPUT

The program accepts ASCII input file. The data may be specified in free format. Currently, the molecular geometry is accepted in Cartesian coordinates. The property data are accepted through another file, which is again an ASCII file. These scalar data may be over a two-dimensional (2D) or three-dimensional (3D) regular grid.

CAPABILITIES

One of the primary requirements of chemists is to visualize molecular structure. This is possible in the package via the three models: ball and stick, stick, and CPK (Corey–Pauling–Koltoun). In the *ball and stick* model, the atoms are shown as spheres and the bonds as cylinders. In the *stick* model, the radius of spheres is reduced to the radius of bonds. This model is widely used for display of large and complicated molecules such as polymers of biomolecules. The *CPK* or *space-fill* model of molecules does away with the bonds and displays atoms as spheres of the corresponding van der Waals radii. If present, the scalar data over a three-dimensional grid can be used to "texture" the van der Waals surface (i.e., texture the CPK model with the given property). A user sometimes needs scaled-up as well as scaled-down textured van der Waals plots: such a facility is provided by the present package.

The data over a two-dimensional grid (or a plane perpendicular to standard axes in the three-dimensional grid) could be visualized in many possible ways. One can have a pixel plot showing color variation (proportional to the function values) over the said plane, or one could look at the contours in the plane. It is also possible to visualize gradients in the plane, although these are evaluated numerically. The gradient vectors are color coded to represent their magnitude. All the above objects—textured plane, contours, and gradients—can be superimposed on one another, to gain a better feel for the variations in the data. The textured plane can also be viewed as a three-dimensional object, with the function value taking the third dimension. This is possible with a *mesh plot*, in which the pixel plot is displayed as textured peaks and valleys. Such a plot may be rotated to obtain a better view of the surface.

The investigation of given data over a three-dimensional grid may be carried out by visualization of the following objects, either singly or in combinations:

- Stacked textured planes
- Stacked contours
- Stacked mesh plots
- Gradients over the entire 3D grid
- Chicken wire/wire frame plots
- Constant valued/isovalued surfaces
- Gradients over isovalued surfaces
- Molecule itself, in one of the three models

One cannot overemphasize the utility of contours and isovalued surfaces: these are two of the most widely used property description tools. The Marching Cube algorithm is used for reconstructing contours and isovalued surfaces. The basic idea of the algorithm is to look at a "cube" for which we know the function value at each corner (i.e., a cube/rectangle within the given 3D/2D data grid). The function (i.e., the property) is assumed to be continuous in the region of interest. The 3D/2D grid on which the data are generated should be fine enough to allow an accurate reconstruction of the surfaces/contours. We then compared the corner values with the value of the surface of interest. For each cube with at least one corner value above and one corner value below the surface value, we know that the surface exists inside the cube. We detect all such cubes in the given data and construct the required surface out of it. For a more detailed discussion, reference may be made to Bloomenthal[15] and Lorenson and Cline.[16]

Apart from the above-described features, the package contains a critical point guessing routine as well as a gradient path routine. With these, one may be able to carry out a critical point analysis given the data over a 3D grid. The critical points (CPs) $\mathbf{p}$ of a three-dimensional scalar field are defined as those where $\nabla f_{\mathbf{p}} = 0$. The nondegenerate CPs in the three-dimensional case are (3, +3) a minimum, (3, −3) a maximum, and (3, −1) as well as (3, +1) saddles. A classification of the CPs is given in terms of the eigenvalues λ_1, λ_2, λ_3 of the corresponding Hessian matrix $H_{ij} = \partial^2 f / \partial x_i \partial x_j |_{\mathbf{p}}$. Here, the notation (r, σ) stands for the rank r and signature (excess of positive eigenvalues over the negative ones), σ (for a lucid introduction to topographical concepts see Stewart[17]). The CPs with at least one vanishing eigenvalue are called *degenerate*.

The package also has a facility for creating PostScript as well as Printer Command Language (PCL) files for the hardcopy reproduction of images, suitable for printers sup-

porting the respective languages. UNIVIS also allows a slide show presentation of prestored images.

NOVELTIES

In the present version, the ray-tracing technique is not employed for creating light and shade effects. Ray-tracing techniques[18,19] produce realistic images that include the effects of shading, shadows, transparency, and reflections. The technique can be briefly summarized as follows: starting from the viewing position a ray is passed through each pixel in the viewing plane and then traced back into the objects defined in the image. The ray can either strike one of the objects in the scene or pass through the scene. If the ray strikes an object, this ray can then be reflected and refracted, generating several new child rays. These rays are then traced like the partner ray, creating more rays and resulting in a cascade effect. The intensity of the corresponding pixel is then set by determining all of the contributions from the parent and all the child rays. Usually the number of generations of child rays that can be generated is limited, since after several generations their contributions become negligible. However, the amount of computation is prohibitively large and requires considerable time. We have, therefore, refrained from implementing such a technique, which has enabled us to achieve a faster rendering of surfaces. The images shown in Color Plates 1–10 were generated on an 80486DX2/66-MHz computer, each within less than 1 min. It should be noted that the image size is 768 × 768 pixels. A typical ray tracer package takes anywhere from 5 min to 10 hr to render a scene, depending on its complexity. But UNIVIS renders any complicated structure or ensemble of objects within a minute or two. The rendition timings for the pictures reported in this work are less than 2 min each. The input data generated over a three-dimensional grid contained ~500 000 points. The restrictions on the number of points are dictated by the availability of memory.

To enhance the presence of the third dimension, UNIVIS has a facility for displaying gray-shaded planes in the background. This simulates a feeling of the ensemble as though kept in a room with light from one side. Such a facility is useful for creating presentation slides. Furthermore, the images can also be gray scaled, for taking black-and-white photographs.

Another novelty of the package is the inclusion of transparency effects. To the authors' knowledge, packages on the PC platform that give such a facility are scarce. UNIVIS employs pinhole-type transparency. Usually, the effects of transparency are obtained by suitable mixing of colors of the said surface and the colors of the objects below. However, when the palette size is restricted (which is true in the present case), such a scheme may not yield the best results. Hence, to obtain transparency effects, the said surface is assumed to be a fine wire mesh, with a varying density of holes (depending on the degree of transparency). Such an effect could be achieved by texturing various dither patterns onto the said surfaces. The objects below the "transparent" surface are visible through the holes in the surface. Such a facility is useful, especially while visualizing complicated surfaces and/or multiple objects. The attribute, degree of transparency, for an object determines its opacity/transparency; the larger the value, the higher the transparency. The package also allows truncated isovalued surfaces at the specified standard planes (parallel to either coordinate axes). It hence becomes possible to visualize objects that are completely encompassed by the said isovalued surface.

The package also permits the user to change the color-mixing scheme and modify function and gradient ranges. The color-mixing scheme can be modified by the user to suit specific needs. The colors on all the objects change instantaneously, allowing the user to select the proper color combinations. To concentrate on a specific range of the function or the magnitude of gradients, the user can suppress the rest of the data by "doctoring" the function as well as gradient ranges. These ranges map the function values and gradient magnitude values to the color range. By modifying these ranges, any part of the data may be enhanced or suppressed. Although the package tries for equicolor distribution, clustering of values in a particular portion of the range may happen. This range-modifying facility is particularly useful in such cases.

ILLUSTRATIONS OF MOLECULAR PROPERTIES

A comprehensive molecular properties package, UNIPROP,[20] developed in our laboratory enables efficient evaluation of a variety of molecular properties at the ab initio level. These properties include molecular orbitals, electron density in position (ED) and momentum space (EMD),[21] electronic moments, and molecular electrostatic potential (MESP) and field.[22] Properties useful for throwing light on the localization of electrons in molecules, namely electron localization function (ELF) and Laplacians of ED and EMD, are also available. Topographical characterization of MESP, ED, and EMD are unique features of UNIPROP. Many of these properties are available on a parallel platform as well. Use of thee properties is made in Color Plates 1–10.

FUTURE PLANS

The package currently operates in an off-line fashion, but it may be coupled with a fast molecular electrostatic potential (MESP) routine, for example, for on-line generation of the minimal surfaces for anions.[23,24] Similarly, simultaneous visualization of two different properties may be undertaken: for example, texturing MESP on a constant density surface such as the one expounded by Bader.[25] Such utilities may be useful to chemists for making predictions regarding reactivity patterns. Apart from the present static graphics, animated sequences of reaction dynamics will also be implemented. This will show the path of the reaction in progress, offering better insights about the mechanism. The package will be ported to the X-Windows platform in the near future.

SUMMARY

The goal of the present work is to provide a package for visualization of 2D/3D data at a low cost. UNIVIS achieves

that target to a large degree. The speed of surface generation and implementation of various levels of transparency for surfaces are the highlights of UNIVIS. The package is meant to be used not only by chemists, but by those needing visualization of 2D/3D scalar data. The package in no way hinders such an attempt. One can easily employ UNIVIS for scientific visualization in such fields as aerodynamics, fluid dynamics, physics, mathematics, biology, as well as medical imaging, in which many scalar or vector data are generated. Furthermore, with its novelty and speed, visualization using UNIVIS can be elevated to a level at which it becomes a research tool, rather than a communication tool. It is hoped that UNIVIS finds its proper place in the theoretical chemist's toolbox.

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