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QMView: A computational chemistry three-dimensional visualization tool at the interface between molecules and mankind

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QMView is designed to facilitate the visualization and interpretation of quantum mechanical data. Capabilities include display of chemical structure, animation of quantum mechanically determined vibrational modes, and depiction of electronic properties and three-dimensional molecular orbitals. QMView has a user-friendly interface that allows users to interactively manipulate many features of the molecular structure and/or property, including positioning and structure representation, via mouse-activated dialog boxes. Although the interface allows input from results of any of the popularly used quantum mechanical software, we have focused on GAMESS,[1,2] a widely distributed quantum chemistry code. QMView has been designed with the special feature of working in distributed mode with GAMESS, the latter running on a supercomputer, the former running on a Silicon Graphics platform. Ancillary programs provide a method of obtaining output of graphic images in various media, including hardcopy, PostScript files, slide, and/or video. These and other original features discussed in this article provide a graphic interface that is unique compared to others that are currently available. Examples of images produced by QMView are presented.

Keywords: quantum mechanics, interactive computer graphics, vibrational modes, molecular orbitals, electrostatic properties, SGI workstations.

INTRODUCTION

Utilization of computationally derived chemical and physical properties has vastly enhanced the success of experimental ventures into the creation of designer molecules of technological and medicinal importance. Rational drug design and novel nanomolecular materials would be complete fantasies if not for the atomic-scale insight provided by computational chemistry. Because of the high demand for pharmaceuticals and composite materials to display a special uniqueness of action or efficiency in response, the tightness on specific structural tolerances and hence the degree of complexity in these molecular blueprints are increasing at a rate manageable only by advanced computing methods (e.g., massive parallelization, or ultrafast vectorization). Despite the extraordinary abilities of modern hardware technology and coding methods to manipulate the raw data, the rate-limiting step in harmonizing the intricacy and precision required to push forward these chemical frontiers ultimately comes down to the process of human–machine information transfer. Along this line, words are to scalar processing what images are to parallel processing, thus, the development of versatile and facile three-dimensional visualization tools is the key to any successful human interface in this endeavor.

Quantum Mechanical View (QMView) has been designed to provide the chemist with an expansive array of molecular perspectives. In addition, specific tutorials within QMView open up exceptional educational avenues for instructors. Indeed, QMView is an integrated visualization package that capitalizes on the increased capabilities of new graphics systems to profile three-dimensional molecules not only by their common ball-and-stick or space-filling models, techniques that convey limited geometrical information, but also by molecular orbitals, electron densities (differential and absolute), electrostatic potential gradients, vibrational normal modes, or regional hydro- or lipophilicity. Each profile can be adjusted, updated, and presented three dimensionally, fully colorized and in real time. All of these capabilities greatly facilitate the analysis of data produced from quantum mechanical techniques.

Color plates for this article are on pp. 61.

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OVERVIEW OF PROGRAM

QMView is written primarily in C, using the Silicon Graphics, Inc. (SGI) GL graphics library. Several of the quantum mechanical components (e.g., the orbital plotting procedure) are written in FORTRAN and interfaced with the main structure via file I/O. In addition, QMView can act as a direct interface to the widely used quantum chemistry package GAMESS,[1,2] with the latter is running on a supercomputer, via UNIX sockets written in C and called from within GAMESS.

User interface communication is performed primarily through mouse-activated icon boxes. In interactive mode, the user is initially presented with a screen as shown in color plate 1. The five large icon boxes give basic demonstrations of QMView capabilities, which include (1) display and manipulation of molecular structure, (2) display of quantum mechanically generated vibrational motions, (3) display of quantum mechanically generated electron densities, molecular electrostatic potential, and density difference maps, (4) display and manipulation of quantum mechanically generated molecular orbitals, both two dimensional and three dimensional, and (5) additional features explained in detail below. The icon on the very bottom of the QMView interface, labeled "research," is intended for user-generated input for any of the above-listed capabilities.

Activation of any of the interface icons will pop up a secondary interface intended for direct manipulation of the molecular system and associated properties. This interface is illustrated in Figure 1. Description of each capability and individual features are addressed in turn below.

Display and manipulation of structure

QMView will display three-dimensional molecular structure when given very basic information, which includes the number of atoms in the molecule, the number of different kinds of atoms in the molecule, and a listing of each atom followed by its Cartesian coordinates. There are a number of structure descriptors that the user can then choose from to tailor the structure to individual user requirements. These include (as seen in Figure 1, left-hand column) labels for control of each individual atom type and bond characteristics. Clicking these labels allows the user to choose (1) individual atom color and (2) radius of each atom; the user may (3) display characteristics of the atom, including circles, beach balls, lighted spheres, transparent spheres, dots, or as virtual atoms, (4) label the individual atom names and numbers, and (5) change the characteristics of bonds from the following choices: (a) no bonds, (b) lines, (c) color-coded lines, (d) lighted cylinders, or (e) color-coded lighted cylinders. An option also exists, via picking, for creating bonds, deleting bonds, and labeling individual bond lengths and angles.

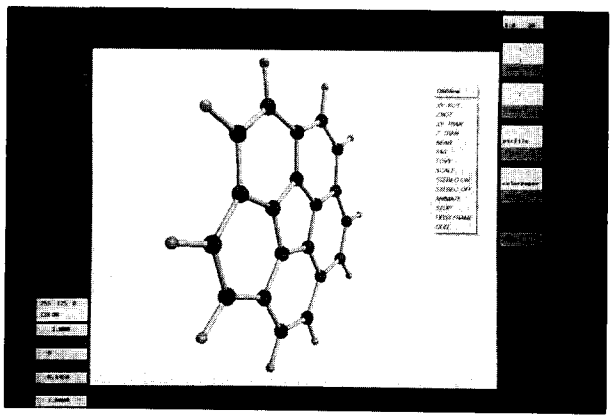

Figure 1. The second layer of the graphical user interface of QMView. This layer may be accessed directly with command line arguments, thereby bypassing the first layer graphical user interface. Various functionalities are depicted as icons along both left and right sides, as well as via a list that pops up from the right mouse button.

The labels displayed in the bottom left-hand portion of the secondary user interface control, in more detail, the labels displayed in the top left-hand portion. Options include (1) more specific selection of color for any of the above-mentioned features, (2) explicit control of the radius of individual atoms and/or bond thickness on selection of the particular atom or bond, and (3) selection of a cut-off value that gives a maximum separation between atoms for connectivity. Alternatively, the user can include the equivalent keywords and/or specific molecular connectivity information within the input file.

Transformation menus

The transformation menus are not initially visible. They can be accessed in two manners. One way is via the right mouse button, in which case the menu comes up much as a pop-up menu. Additionally, the menus can be popped up on the bottom of the screen by using a toggle switch. The menu items include x, y, and z rotation and translation, controls over the near and far clipping plane, scaling of the image, stereo projection of the image (provided the hardware is available), and control over the field of view. In general, QMView displays the image with a perspective projection; objects that are closer in the z direction appear larger than those objects further away. An orthogonal projection may be approached by decreasing the field of view, which is done by selecting the appropriate menu item.

Display and manipulation of vibrational frequencies

QMView can display, in real time, the vibrational frequencies that are calculated from quantum chemical calculations. The input is the same as described above for display of molecular structure, with the inclusion of the specific vibrational frequencies and corresponding modes as extracted from a quantum chemical calculation. The key display options include (1) selection of which vibrational mode to display, (2) control over the number of frames for which to display the vibration, for one vibrational period, and (3) a control over the smoothness and amplitude of the motion.

Display of electron density and associated properties

Given the basic input described above for the display of structures, with the inclusion of either an electron density

grid or a molecular electrostatic potential grid (from a previous quantum mechanical calculation), QMView will display the molecule and associated contours. A set of menus will be appended to the standard molecular control menus on the left-hand side of the secondary interface, according to the contour values. Any combination of these contours can be displayed.

The display of contours can be in terms of two-dimensional planes passed through the three-dimensional structure, or, in terms of three-dimensional (3D) contours of either net, solid or transparent surfaces. Figure 2 illustrates the total electron density of the anthracene photodimer, lepidopterene, in terms of a net surface, as calculated using the Density Functional Theory software package, DMol.[3]

The solid surfaces are generated via the Marching Cube algorithm.[4] In addition, one can create a transparent 3D surface, with a superimposed two-dimensional plane of particular contours. All transformation features as described for molecule manipulation work as well as for manipulation of the molecular orbitals.

Display of molecular orbitals

QMView includes a module that allows calculation of molecular orbitals from the wavefunction of a previous quantum mechanics calculation. The input for this module includes the basic molecular structure information as described in the above features, along with explicit information provided by the quantum chemical package concerning the details of the basis set and molecular orbitals for the specific molecule. QMView then draws contour plots of the individual molecular orbitals as expanded in the basis of *s*-; *p*-; and *d*-contracted Cartesian Gaussian[5] functions, or in the basis of *s* and *p* Slater[6]-type orbitals. Display characteristics are similar to choices described above for electron density grids, including a choice of (1) wire surface, (2) solid surface, or (3) transparent surface.

Color Plate 2 depicts the highest occupied, bonding molecular orbital (HOMO) superimposed on an electron density surface of the C_{20} fullerene molecule.[7] The HOMO is depicted with red and green surfaces indicating negative and positive surface values, respectively; the electron density surface is shown in blue. Calculations were performed using the Local Density Approximation.[8]

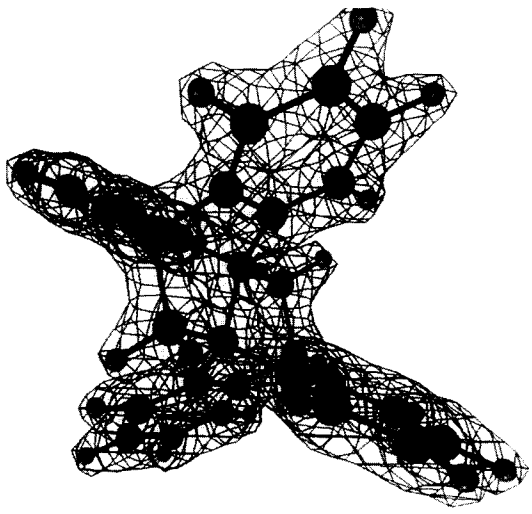

Figure 2. Depiction of the total electron density of lepidopterene as calculated using Local Density Functional Theory as implemented within DMol.[3]

Additional features

QMView has been programmed to run in a distributed mode with other platforms. In distributed mode, a remote machine, such as a Cray C90 or an Intel Paragon supercomputer computes the information that QMView displays in real time. The connection between the SGI and the remote machine is via UNIX sockets written in C and called from within the quantum mechanics package. Running QMView in distributed mode requires information such as the name and port number of the remote machine. QMView prompts the user for all necessary information. Once the information is provided, QMView displays the first configuration that is produced by the quantum mechanics package, along with (optionally) two inset *xy* graphs, one of which monitors the energetics as a function of the calculation iteration, and the other of which monitors the root-mean-square of the minimization procedure with respect to geometry as a function of calculation iteration. This feature allows the user to monitor and check on long quantum chemical calculations to make sure it is proceeding correctly.

A second added feature to QMView is a module consisting of educational chemistry tutorials. The purpose of these tutorials is meant for use in a classroom environment for teaching of basic chemical phenomena. This module is very small now, but is currently being expanded. Examples of the tutorials within this module are as follows.

Interaction of basic atomic orbitals. Invoking this tutorial allows animation of basic molecular orbital formation from atomic orbitals. Examples include *s*-orbital interactions, *s–p* orbital interactions, *p–p* σ and π-orbital interactions, *p–d* and *d–d* orbital interactions.

Structure of DNA. This tutorial was actually constructed for a classroom situation at the University of Davis (Davis, CA, USA) under the direction of J. Keizer, in order to illustrate the detailed structure of DNA for a class of several hundred students. Invoking this tutorial launches the user into a structural tour of a small coil of helical DNA,[9] including dimensional analysis of the stereochemistry of the various base–base combination structures, and the base–sugar backbone structure. Views include color-coded ball-and-stick and space-filling representations. Color Plate 3 illustrates a space-filling view of a segment of DNA.

OUTPUT CAPABILITIES

QMView uses the San Diego Supercomputer Center (SDSC) "vpr" program[10] to make hardcopy outputs of structures on color copiers and film. QMView dumps an SGI ("rgb") image file to disk and "vpr" converts the raster image to the form required by the particular output device. The SDSC image tools may easily be incorporated

in order to produce output on, for example, PostScript printers via the standard UNIX "lpr" utility.

QMView also has several "camera control" options for making presentation videos (e.g., for the classroom or for seminar purposes). Rotations, translations, scaling, and clipping may be programmed along with, for example, dynamic or vibrational progression. For example, a user may choose to display a vibrational mode while rotating the structure simultaneously. They may then select the angle of rotation about one or more coordinate axes and also choose the number of vibrational iterations to skip over for each frame of film or tape. After each frame has been recorded, a "checkpoint" file is written that saves all the characteristics of the vibrational animation (transformation matrices, colors, bonds, etc.) so that the user may stop recording and continue at another time. When QMView is restarted using the same input files, the checkpoint file is read automatically and the last configuration saved appears on the screen.

Using the "animate" feature, a user may predefine, within the input file, vector movements for all atomic positions where each vector set defines some type of motion (e.g., along an axis, diagonal, etc.). Applications of this feature include (1) the illustration of the superposition of conformers, and (2) the illustration of motion along a quantum mechanically calculated reaction path.

When all the motion options are selected, the user may select the "GO" menu item and the recording will proceed automatically. From our experience, we are able to record up to about 1000 NTSC resolution frames per hour to a video disk, depending on the size and type of data being displayed and on the particular SGI hardware being used. At the SDSC, nonproprietary programs are available for controlling Sony laser disks directly from SGI workstations. The "record" command is called from within QMView via the UNIX library routine "system" after a frame has been rendered and may be modified to suit a particular site.

FUTURE DIRECTIONS AND CONCLUSIONS

Although the era of high-performance computing has allowed phenomenal capabilities for computing larger and more complex problems at ever-faster speeds, the scientific visualization of the complex data and the ability to teach fundamental chemical principles visually have captured the imaginations of scientists and educators in productive ways. QMView will continue to be developed via collaborations in both research and education. The package is being distributed with the companion package, GAMESS, a widely distributed quantum mechanical package, on a nonprofit basis although a stand-alone version plus a manual is also available by contacting the authors.[11] Beta test sites have already been successfully established at the University of California at San Diego (San Diego, CA, USA), ISU, and two industrial research sites. The currently available version is for the SGI platform, although future plans include a port to OpenGL so that other workstations can be used.

ACKNOWLEDGMENTS

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REFERENCES

1 GAMESS (General Atomic and Molecular Electronic Structure System) is an ab initio quantum chemistry package that allows study of chemical systems containing atoms through radon from the simplest closed shell case up to a general MCSCF case, permitting calculations at the necessary level of sophistication. For detailed information on this code and its parallel implementation, see references given in Ref. 2.

2 Schmidt, M.W., Baldridge, K.K., Boatz, J.A. Jensen, J.H., Koseki, S., Gordon, M.S., Nguyen, K.A., Windus, T.L., and Elbert, S.T. *QCPE Bull.* 1990, **10,** 52; Schmidt, M.W., Baldridge, K.K., Boatz, J.A., Elbert, S.T., Gordon, M.S., Jensen, J.H., Koseki, S., Matsunaga, N., Nguyen, K.A., Su, S., and Windus, T.L. The General Atomic and Molecular Electronic Structure System. *J. Comput. Chem.* 1993, **14,** 1347

3 VernonClark, R., Battersby, T., Gantzel, P., Chadha, R., Baldridge, K.K., and Siegel, J.S. Pi-sigma-pi through-bond coupling and "long" C-C single bonds. *J. Am. Chem. Soc.* 1994 (in press); DMol is a program developed at Northwestern for quantum mechanical calculations using Local Density Functional Theory (Delley, B. *J. Chem. Phys.* 1990, **92,** 508)

4 Lorensen, W.E. Marching cubes: a high resolution 3D surface construction algorithm. *Comput Graphics* 1987, **21,** 163; We would like to acknowledge Jonathon Shade, SDSC, and Michael Bailey, SDSC, for their help in the coding and implementation of these methods into QMView.

5 Boys, S.F. *Proc. R. Soc. (London)* 1950, **A200,** 542; Shavitt, I. In: *Methods in Computational Physics,* Vol. 2, John Wiley & Sons, New York, 1962, p 1

6 Slater, J.C. *Phys. Rev.* 1929, **34,** 1293; Slater, J.C. *Phys. Rev.,* 1930, **35,** 509

7 Taylor, P.R., Bylaska, E., Weare, J.H., and Kawai, R. C_{20}, fullerene bowl, or ring? New results from coupled-cluster calculations. *Phys. Rev. Lett.* 1994 (in press)

8 Kawai, R. Unpublished software employing the Kohn–Sham density functional theory (Hohenberg, P. and Kohn, W. *Phys. Rev. B* 1964, **136,** 864; Kohn, W. and Sham, L.J. *Phys. Rev. A* 1965, **140,** 1133)

9 The coordinates used to generate this DNA tutorial were extracted from the Protein Data Bank. The specifics on this are as follows:

Deoxyribonucleic acid 02-Mar-92
DNA$ (5′-
$D(*CP*GP*CP*AP*AP*AP*TP*TP*TP*GP*CP*G)-3′)

Edwards, K.J., Brown, D.G., Spink, N., Skelly, J.V., and Neidle, S. Molecular structure of the B-DNA dodecamer D(CGCAAATTTGCG)2; an examination of propeller twist and minor-groove water structure at 2.2 angstroms resolution. *J. Mol. Biol.* 1992, **226,** 1161

10 Nadeau, D.R., Elvins, T.T., and Bailey, M.J. Image handling in a multi-vendor environment. *IEEE Computer Society Press Reprint,* 1991, 276.

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