Visualization of Molecular Quantum Dynamics – A Molecular Visualization Tool with Integrated Web3D and Haptics

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Abstract

The Department of Chemistry and the School of Informatics at the University of Wales, Bangor are working together to create tools for the visualization of molecular quantum dynamics. This paper presents the results of our initial work. A prototype Molecular Visualiser (MV) application has been developed based on Web3D standards, plus extensions for support of haptic interaction. MV provides the user with visualizations of molecular systems, potential energy surfaces, and wavepacket dynamics. These can be displayed in a web browser using VRML, or be delivered to a virtual environment in which haptic properties have been assigned based on the molecular dynamics of the system. The use of MV for both research and teaching is discussed.


Keywords: Visualization, Molecular Quantum Dynamics, VRML, Haptics

1 Introduction

Chemists rely heavily on visualization as a key to understanding chemical processes. Geometrical structures are described pictorially in terms of their equilibrium structures and reactions are visualised as a scheme. This type of approach has allowed the chemist to gain great insight into complicated chemical processes that would otherwise impede progress in this field. However, if the chemist turns to quantum mechanics to gain a more detailed description of some chemical process this intuition can easily become lost in the mathematical formalism underlying the theory. This intuition need not be lost. In much the same way that a chemist uses visual reaction schemes to understand complex chemical processes, the chemist can study the time evolution of quantum dynamical (QD) wavepackets on the complicated potential energy surfaces that govern their motion. Interpretation and understanding the detailed dynamics of quantum molecular systems can be achieved by visual analysis of wavepacket dynamics. The initial phase of this work, however, has concentrated upon molecular rendering.

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Dreiding and Corey-Pauling-Koltun (CPK) mechanical models have been routinely used in the form of model kits, to represent 3D molecular structures for several decades [Macmillan 2004]. However, the advent of molecular graphics has enhanced the accessibility of molecular modeling techniques, and assisted in the analysis and interpretation of the underlying theoretical calculations. Both mechanical and molecular graphics-based models are, however, only our own macroscopic interpretations of the quantum universe. Even models obtained from experimental techniques employing Scanning Probe Microscopies (SPMs) [Samori 2004] such as Atomic Force (AFM) or Scanning Force Microscopy (SFM) [Binnig et al. 1986] that allow an atomic probe to ‘feel’ an individual molecule, do not paint a wholly realistic picture of the quantum universe, as false colour and visual conventions (e.g. CPK) of molecular surfaces must be applied to present the experimental data.

Molecular graphics models are commonly represented using ‘stick’ or ‘space-filling’ representations, analogous to the aforementioned Dreiding and CPK mechanical models, together with other subtle variations on these two basis types such as ‘tube’ and ‘balls and stick’. The inclusion of shading and lighting effects, coupled with an element-specific colour scheme provide more realistic graphics. For large molecular systems, the sheer number of atoms can result in a cluttered picture and is often limited by the power of the system’s graphics card. The visualization of protein and enzyme structures, such as dihydrofolate reductase [Bolin et al. 1982], can be enhanced by the ‘ribbon’ representation in which the backbone (hydrogens omitted) is depicted as a set of cylinders (α-helices), flat arrows (β-sheets), or tubes (no regular structure).

Quantitative information such as simple geometric properties, or Ramachandran maps [Ramachandran et al. 1963] for conformational analysis, can be easily obtained from molecular graphics, but are difficult if not impossible to obtain from standard mechanical models. However, the ease with which mechanical models can be manipulated and viewed in three dimensions has not yet been surpassed by standard mechanical models, even though an impression of the 3D structure of a molecular graphic can be obtained via depth cueing, the use of perspective, or stereo images. In this respect, the use of virtual environments (VEs) has been touted as being suitable for the interaction with a computer generated molecular model, in much the same way that a standard model kit can be manipulated, strengthening the links between the quantum universe and the macroscopic world. A VE will cater for not only 3D visualization, but sophisticated interaction via force-feedback, or haptic, devices.

This paper describes the first stage of our development of an environment for the visualization of Molecular Quantum Dynamics. The result of this work is a prototype Molecular Visualiser (MV) virtual environment, which includes novel tools for the visualization of potential energy surfaces, and wavepacket dynamics.
dynamics. One of the uses of MV is as a cost effective tool for undergraduate chemistry students to use, offering support for both visualization and haptic interaction. MV will parse a text file containing a structural description of a molecule, calculate the molecular properties, and generate a VRML 97 scene graph to allow web-based visualization of the given molecular system. For haptic interaction, we make use of a Reacinh Display [Reacinh Technologies], which allows for the co-location of stereoscopic renderings of the molecule with a PHANTOM Desktop haptic device [Sensible Technologies] (see Fig.1). MV will assign appropriate haptic properties to the molecule based on molecular dynamic calculations. The aim of MV is to provide most of the educational functionality of leading commercial molecular modeling software packages.

2 Background

There has been considerable interest in the use of 3D environments for scientific visualization, and several applications for chemistry can be found in the literature. A good example is the Vienna ab initio simulation package (VASP) data viewer, a desktop 3D visualization application for the analysis of valence electronic structure information [Terrberry et al. 2002]. VASP is being extended to support immersive environments such as the CAVE. CAVEs have already been exploited for the visualization of protein surfaces using structural representations, e.g. space-filling, solvent-accessible surface, molecular surface and the alpha complex algorithm [Akkiraju et al. 1996]. The docking of chlorpromazine and mepacrine with the trypanothiophane reductase of Trypanosoma cruzi, a parasite that causes Chagas’ disease was also achieved using a CAVE system [Wood et al. 1996]. A combination of visualization and molecular dynamics (MD) is often employed within state-of-the-art chemical immersive set-ups, as the physical properties of the model can be manipulated in real-time, allowing the user to perform a ‘virtual experiment’. A CAVE system is also one of the constituent components of the Virtual Biomolecular Environment (VIBE), which was successfully used to steer a cyclic urea compound into the active site of the HIV protease [Cruz-Neira 1996]. A computation performance of 15 frames per second, and a rendering performance of 48 frames per second have been obtained with and without MD, on a 64 node SP2 parallel computer, illustrating the huge computational demands upon merging of real-time MD simulations with an immersive display. More recently, a CAVE facility based entirely on Java3D software has been developed, including chemistry-related applications [Burleigh et al. 2003], thus showing that Web3D technologies can scale from low to high end configurations.

High end systems that have been used for chemistry visualization sometimes include support for haptic devices. A well known example is Project Grape [Ouh-Yong et al. 1988; Brookes et al., 1990], which was the first to demonstrate the usefulness of haptic interfaces for the perception of force fields, and in molecular docking. The potential of using haptics for the teaching of structural molecular biology has also been reported [Sankaranarayanan et al., 2003]. Early results indicate that haptic feedback should provide an intuitive learning interface.

Other solutions focus just on 3D visualization for chemistry, and do not have the associated costs of setting up and maintaining a sophisticated immersive VE. Web3D technologies such as X3D and the ISO-standard Virtual Reality Modeling Language (VRML 97) fall into this category. Chittaro and Serra [2004] have summarized the general educational benefits that can be obtained through appropriate use of Web3D. Our hypothesis is that these benefits, which include knowledge-building experiences and the ability to analyze phenomena from different points of view, will help an undergraduate chemistry student to more quickly learn and understand key concepts such as molecular dynamics.

VRML has already been used successfully within chemistry. For example, Casher et al. [1998] show that in principle any computed molecular surface can be represented in VRML. Their work includes examples that use animation, data mining techniques, and descriptions of laboratory instrumentation. Leach and Gilbert [1999] demonstrated the first use of VRML for visualizing molecular dynamics trajectories. Work is also underway to develop the Chemical Markup Language (CML), which allows a XML marked up molecule to be displayed in a variety of different ways [Murray-Rust 2003]. CML can easily be converted to X3D and other formats by using an appropriate XML style sheet [Polys 2003].

Another alternative is Molecular Inventor, an open source toolkit that facilitates the rendering and interaction of chemical systems [openMOIV]. Molecular Inventor is a set of extensions of Open Inventor and so shares its roots with VRML 1.0. It includes support for atoms, bonds, isosurfaces, 3D contours and labels. However, it is platform dependent (IRIX only) and like VRML 97, has no support for haptics.

3 Molecular Visualiser (MV)

The implementation of MV has been based on Web3D technologies to guarantee both cost effectiveness and good availability within the University’s computer laboratories. VRML has been used by MV to deliver a 3D molecular representation to any standard PC. MV has also been designed to support haptic interaction within a Reacinh Display, to provide the student with an exciting environment for carrying out virtual experiments – see Fig. 1. The Reacinh API is based on the VRML 97 scene graph, providing new nodes that allow haptic properties to be associated with geometry. The core software for calculating the molecular system has been written using Java.

In collaboration with lecturers from the Chemistry Department, a list of design criteria for MV was created:

- The ability to input the structure of a molecule in Cartesian coordinates.
- To deduce which atoms, if any, are bonded to one another.
- To diagonalise the initial inertia tensor, obtaining the principal axes and moments of inertia.
- To rotate the molecule so that it lies along the principal coordinate frame.
- To calculate the space group and rotor type for a single molecule system.
- To generate separate UTF-8 / ASCII text file containing a description of the molecular system for both standard VRML-compliant browsers and the Reacinh-API compliant Reacinh Desktop workstation.
These features are the minimum requirements to create an effective tool for a chemistry undergraduate student. Furthermore, MV should:

- Allow the student to freely manipulate and rotate the molecular system.
- Describe the molecular system with a range of rendering options such as ‘stick’, ‘balls-and-stick’, ‘tube’, and ‘space-filled’.
- Incorporate a set of labelling options commonly found in commercial software.
- Allow the student to perform a wide variety of geometrical measurements upon the system, such as bond length/interatomic distance, three-body bond and four-body torsional angle;
- Incorporate a dynamical model for realistic rotation and translation of the molecule based upon the inertia tensor.
- Incorporate haptic properties.
- Allow the user to interact with the potential energy and wavepacket surfaces;

All of the required and optional features listed above have been successfully implemented in the first version of MV described in this paper.

3.1 Structural Input

The inputting of molecular structures is non-trivial as there is a wide variety of varying file formats that both standard commercial and in-house software employ, ranging from internal coordinates (e.g. Z-matrices) for ab initio and semi-empirical quantum mechanical packages such as Gaussian and Mopac; to fractional coordinates (e.g. .xil) based on a given unit cell for crystal structures, surfaces and 3D amorphous solids; and standard Cartesian (x, y, z) coordinates (e.g. .car, .pdb, .mol) for both small-molecule and macromolecular systems. As VRML 97 and the Reachin API both employ a Cartesian coordinate space, the input of structural data in the form of Cartesian coordinates was chosen as the molecule (scaled to be visualised correctly within the Reachin environment) can be directly incorporated into the VRML-based applications without the need of further interconversion programs. Figure 2 shows the interface for MV File Input Parser.

Atom/bonding connectivity is not explicitly defined, and so all covalent bonds must be assigned independently. This is achieved as follows:

I. if \((\text{atoms} + \text{heteroatoms}) > 255\)
   a. if \(0.4 \text{ Å} \leq r_{AB} \leq 1.9 \text{ Å}\),
   b. if \(A\) or \(B\) are hydrogens, the bonded range is \(0.4 \leq r_{AH} \leq 1.2 \text{ Å}\).

II. else if \((\text{atoms} + \text{heteroatoms}) \leq 255\)
   a. if \(0.4 \leq r_{AB} \leq (\text{cov}_A + \text{cov}_B + 0.56) \text{ Å}\)

where \(r_{AB}\) is the interatomic distance between atom A and atom B, and \(\text{cov}_A\) is the covalent radius for atom A, corresponding to half of the distance between two identical atomic nuclei, bound by a single covalent bond. Although ambiguous for Cl, H, Si, C (diamond), S, Ge, Sn, and a few other elements; the covalent radius is difficult to assign correctly for most elements, e.g. O and N, which contain multiple bonds (e.g. O=O and N≡N respectively), thereby necessitating the inference of the covalent
radius from molecules containing X-X single bonds, or from hetero-diatomics, X-Y, where the covalent radius of element Y is known. This approach is based on the method used by the commercial RasMol package and we have obtained results in excellent agreement with values obtained from other sources [WebElements].

An identical rendering scheme to that employed by packages such as RasMol and Chime has been adopted within MV. Most transition metals, and all lanthanides and actinides are rendered as a deep pink, whereas carbon is rendered as light grey. The colours used for the most common elements are given in Table 1. This ensures universality with most commercial and academic chemistry modeling software.

The sizes of the CPK spheres in both “spacefilling” (as used for the molecule in Fig. 1) and “ball-and-stick” (for example, Fig. 4a) models are determined by van der Waals (vdW) radii, the radius of an imaginary hard sphere depicting the atom, usually determined from contact distances between non-bonding atoms in touching molecules or atoms.

Universal data such as CPK rgb-colour, covalent and vdw radii, and atomic mass (for calculation of centre of mass and inertia tensor, see below) that are required for bonding, rendering and generation of vibrational and rotational data, can be quickly retrieved from an internal hash table. The unique IUPAC element symbol is used as the hash key. Table 2 summarises the VRML primitives that are used within MV for the supported molecular renderings.

All DEF nodes are hard-coded, e.g. Transform, Switch, Script nodes, or obtained from the parser, e.g. Material nodes which describe the colour properties of a specific atom or bond, e.g. light grey for carbon, C. A Vector object within the JAVA parser keeps track of whether a specific IUPAC element symbol has been parsed – if the Vector does not contain the element symbol, it is added to the Vector, and a DEF node created, otherwise a USE instance is employed. Similarly, all field names, types and values are hard-coded into all Script nodes.

Changing between the available molecular rendering schemes is accomplished through TouchSensor nodes implemented as a series of menu buttons within the VRML scene. Clicking above a specific button activates a Script node which sends a specific SFFloat value to the whichChoice field of the Switch node describing the molecular structure, e.g. 0 for spacefill, 1 for wireframe, 2 for cylinder, and 3 for ball and stick. A similar approach is also used to toggle the labeling schemes where whichChoice field values of 0, 1, 2 and 3 respectively describe the IUPAC element symbol, line number (both hard-coded from the parser), inertial axes (see below) and the absence of any label.

3.2 Diagonalisation of the Inertia Tensor

The classic equations used to calculate the inertia tensor are presented in the Appendix. Note that products of inertia (equation A5) are often either quoted without the negative sign, or not at all, both of which leads to an incorrect description of the rotational properties of the body (molecule). This can be tested within the Reachin Display environment, leading to either no or partial, incorrect rotational motions when a rotational torque is applied via the PHANTOM device.

### Table 2: Molecular Renderings supported by MV

<table>
<thead>
<tr>
<th>PHYSICAL DESCRIPTION</th>
<th>VRML PRIMITIVES</th>
<th>TRANSFORM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spacefill</td>
<td>Spheres ($r = r_{CPK}$)</td>
<td>Translation Scaling (ball &amp; stick only)</td>
</tr>
<tr>
<td>Wireframe</td>
<td>Indexed Line Set</td>
<td>None</td>
</tr>
<tr>
<td>Capped cylinders</td>
<td>Spheres ($r = 0.15 \text{ Å}$) Open-ended dual-tone cylinders ($r = 0.15 \text{ Å}$, $k = 0.5 \ast$ bond length)</td>
<td>Translation Rotation (bonds only)</td>
</tr>
<tr>
<td>Ball and stick</td>
<td>Spheres ($r = 0.25 \ast r_{vdw}$) Close-ended solid-white cylinders ($r = 0.15 \text{ Å}$, $h = bond length$)</td>
<td>Translation Rotation (bonds only)</td>
</tr>
</tbody>
</table>

Once the molecular structure is correctly parsed, algorithms adapted from an on-line rotational constant calculator [Shattuck 2004] are employed to generate and diagonalise the inertia tensor to obtain eigenvectors corresponding to the principal axes within the principal coordinate frame, and eigenvalues corresponding to the principal moments of inertia. The original atomic coordinates $(x_a, y_a, z_a)$ are translated (see Equations A2 and A4) to new coordinates $(\alpha, \beta, \gamma)$ relative to the molecular centre of mass $(\mathbf{\bar{x}}, \mathbf{\bar{y}}, \mathbf{\bar{z}})$. The symmetric inertia tensor, $\mathbf{I}$, is constructed, and immediately transformed into an upper triangular matrix, to save memory. The eigenvectors, $\mathbf{V}$, and eigenvalues, $\mathbf{\Omega}$, are linked by an eigenvalue equation, given that $\mathbf{I}$ is a real, symmetric matrix:

$$\mathbf{V}^T \mathbf{I} \mathbf{V} = \mathbf{\Omega}$$  \hspace{1cm} (1)

which is solved using the Jacobi method [Mathworld], an iterative algorithm in which the eigenvectors are calculated from a series of matrix multiplications.
The iteration procedure involves the following matrix operation:

$$A^k = T^k A^{k-1} T^k$$

where the angle is selected to force the $i,j$ terms within the matrix $A^k$ to be zero. This is satisfied if

$$\tan 2\theta = \frac{2A_{ij}^{k-1}}{A_{ii}^{k-1} - A_{jj}^{k-1}}$$

The Jacobi method will always converge and yield an accurate solution for positive, zero or negative eigenvalues. Most computational Jacobi routines, such as the ones in MV, employ a threshold approach in which it skips the relatively small off-diagonal terms and operates only on the large off-diagonal terms to save computational effort, with approximately 10\(n^2\) operations needed to obtain convergence of a \(n \times n\) matrix.

All of the required calculations are performed as a pre-processing stage, before visualization of the molecule. The Jacobi method has been implemented within the Java code of the MV File Input Parser. Note that the calculation of the inertia tensor is fast. On a single processor desktop PC, the Jacobi method typically only takes only a few seconds.

### 3.3 Determination of the Molecular Point Group

A set of nuclear coordinates defines certain symmetry for a molecule that is demonstrated by its symmetry operations. The group of symmetry operations define a point group for a molecule. Molecular properties ranging from simple chirality and polarity predictions, to the assignment of symmetry-adapted molecular orbitals and vibrational normal modes can be deduced from the molecular point group. The Schoenflies system is commonly used for the discussion of molecular point groups, and has been employed within MV. The point group is determined using standard matrix transformations to deduce its component symmetry operations, e.g. rotation, reflection or inversion. Again, this stage is carried out before the visualization of the molecule. It is envisaged that the final version of MV will allow the user to visualise the effects of performing the above symmetry operations interactively. This would promote the teaching of both Molecular Symmetry and Stereochemistry, both of which are difficult to visualise using standard plastic model kits.

### 3.4 Geometric Measurements

The abstraction of geometrical data from a molecular model is of quintessential importance to chemical research and education. Aside from the fact that data inference from geometrical data is far more intuitive than from absolute coordinates; bond lengths, bond angles and torsional angles are also an integral part of Z-matrices for the definition of internal coordinates. Geometrical data plays a vital role within molecular mechanics, where the total energy of the molecule, \(E_{tot}\), including bond (\(E_b\)), angle (\(E_\theta\)), torsion (\(E_\tau\)) and other terms, is minimised to obtain the lowest energy molecular conformation:

$$E_{tot} = E_b + E_\theta + E_\tau + E_d + ...$$

where:

$$E_b = \sum k_b (l - l_0)^2$$

$$E_\theta = \sum k_\theta (\theta - \theta_0)^2$$

$$E_\tau = \sum \frac{V}{2} (1 - \cos n\tau)$$

$$E_d = \sum \frac{q_i q_j}{2 \sigma_{ij}}$$

\(k_b, k_\theta, k_\tau, l_0, \theta_0, V, \sigma_{ij}\) are force constants; \(l_0, \theta_0\) are equilibrium values; \(V\) is the torsional barrier with period \(n\).

The distance, \(d\), between points \(A(x_1, y_1, z_1)\) and \(B(x_2, y_2, z_2)\) is defined as:

$$d = |\vec{r}_{AB}|$$

where:

$$\vec{r}_{AB} = (x_2 - x_1)\hat{x} + (y_2 - y_1)\hat{y} + (z_2 - z_1)\hat{z}$$

The angle, \(0 [0, \pi]\), formed by three points \(A(x_1, y_1, z_1), B(x_2, y_2, z_2)\) and \(C(x_3, y_3, z_3)\) is similarly defined as:

$$\theta = \text{arccos} \left( \frac{\vec{r}_{AB} \cdot \vec{r}_{AC}}{||\vec{r}_{AB}|| ||\vec{r}_{AC}||} \right)$$

The torsion (dihedral) angle, \(\tau\) [-π, π], formed by four points \(A(x_1, y_1, z_1), B(x_2, y_2, z_2), C(x_3, y_3, z_3)\) and \(D(x_4, y_4, z_4)\), as shown above in Figure 2.1 can be defined as:

$$\tau = \text{sign} \text{arccos} \left( \frac{\vec{r}_{AB} \times \vec{r}_{AC} \cdot \vec{r}_{BC} \times \vec{r}_{CD}}{||\vec{r}_{AB} \times \vec{r}_{AC}|| ||\vec{r}_{BC} \times \vec{r}_{CD}||} \right)$$

where sign is evaluated as a matrix determinant from the triple scalar product:

$$[\vec{r}_{AB} \times \vec{r}_{BC}] \cdot [\vec{r}_{BC} \times \vec{r}_{CD}] \rightarrow \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}$$

Two conventions exist for determining the sign of the dihedral angle, \(\tau\) [con]. MV employs the convention defined by Klyne and Prelog [1960], where \(\tau\) is positive when measured clockwise from the front substituent A to the rear substituent D, and negative when measured anticlockwise.
touchXXX.isActive andTouchSensor.eventInouts are wired to atomXXX.isActive Script eventInouts, which output the atomic position of that atom to the geometryScript.set_position eventIn, incrementing an internal counter within a Script node that is used to calculate all geometric data needed from Equations 6 to 10. The counter is used to specify which parameters to calculate and display – bond length (2 atoms), bond angle (3 atoms), torsion angle (4 atoms), etc. As previously stated all field names, types, and values are hard-coded (2 atoms), bond angle (3 atoms), torsion angle (4 atoms), etc. as calculated using the methods described earlier in this section. Therefore, wavepackets embody the wave/particle duality of matter, giving the closet analogy possible to a localised particle. Wigner distributions W(q, p, t) where q and p are position and momentum respectively, i.e. the phase space, are frequently used to represent wavepackets in phase space, and are indispensable in describing the dissipative processes of an open quantum system. One approach for studying dissipative quantum systems is via the Caldeira-Leggett (C-L) equation.

In this work, the C-L equation is applied to large amplitude vibrations, e.g. inversion, which can be described by fitting experimental data to a hypothetical Potential Energy Surface (PES). MV allows the chemistry student to achieve a higher level of understanding of the intricacies of a 3D PES, e.g. for reaction energetics and spectroscopy via haptics incorporation. The software provides a front-end interface to allow the specification of the coefficients needed to define a general potential function, and the parameters for the x, and y coordinates such as the minima, maxima and number of points for each respective axis. In-house software from the Chemistry Department also allows a series of files containing wavepacket data to be output at regular intervals. These data can also be parsed by MV and converted into a form which enables the full 3D wavepacket to be visualised and animated. Section 5 contains some examples and further explanation of these types of visualizations.

5 Results

Figures 4a and 4b contain example visualizations of the Vitamin C molecule that have been generated by MV. The user can toggle between the supported molecular rendering styles. The menu system has been implemented as a Heads Up Display (HUD), and includes support for the user to:

- alter the molecular transparency;
- alter the relative size of the CPK radii used within ball and stick mode;
- measure any bond length, bond angle or torsional angle for a given molecular conformation.

During testing, the .pdb structures for a wide variety of both organic and inorganic molecular rotors were obtained from online sources, and inputted into MV. The principal moments and corresponding inertial axes, space group and rotated principal coordinate frame were compared with their counterparts obtained using the original on-line applications. After allowing for the different eigenvalue and eigenvector orderings, quantitative agreement was achieved between MV and the on-line application.

The inversion mode in cyanamide (N≡C-NH₂) can be characterized by a non-periodic double well potential function of the form V(q) = V₁q^2 + V₂q^4. An example PES of the form z = x^2 – y^2 is depicted in Figure 5, which can be probed using the Reachin environment, with haptics providing additional sensory information, particularly regarding the curvature of the PES. The
PES surface can be described by a combination of PointSet, IndexedLineSet and IndexedFaceSet nodes, where the Coordinate node contains a uniform grid of \((x, y, z)\) tuples. Well-defined IndexedFaceSets are solely employed for the haptic description of the surface.

An initial Gaussian shaped Wigner function for the cyanamide inversion is illustrated below in Figure 6(a), which undergoes rapid energy equilibration with the environment, followed by tunnelling, Figure 6(b), of the wavepacket from the first well into the second. The population of the second well increases, Figure 6(c), until equality with the first well is achieved.

Key-frame animation of wavepacket dynamics is accomplished using a combination of a TimeSensor node which acts as a clock, and a CoordinateInterpolator node, which describes the evolution of the wavepacket surface as a function of time. The animation can be controlled via a remote control (e.g. play, pause, stop etc.) within the menu.

### 6 Conclusions and Future Work

We have developed a cost effective tool to assist with the visualization of molecular quantum dynamics. As well as the research application, this tool has great potential for undergraduate chemistry teaching. The visualization of molecular systems, potential energy surfaces, and wavepacket dynamics can be delivered to any web browser with a suitable VRML 97 compliant plugin. Although a wide variety of molecular structure representations, animated reactions, and surfaces have been previously published using both VRML 1.0 and VRML 97, enhanced scripting and multimedia capabilities have been employed in our work to provide a high level of functionality within MV, including several novel features. Further, we can also utilise the Reachin Display environment, which is affordable to the majority of Chemistry Departments, to combine the use of haptics with 3D molecular visualizations. Initial results also indicate that our hypothesis that by using such tools, an undergraduate chemistry student will more quickly learn and understand key concepts such as molecular dynamics is correct. However, further work is needed to verify this claim by testing the use of MV in the forthcoming academic year.

The next phase of work will focus on the extension of support for wavepacket visualization and haptic interaction. Results to date augur well for the use of such tools in this field of chemistry. From a technology perspective, an open source X3D based haptic scene graph API called H3D has recently been released [SenseGraphics]. New and cheaper stereochemical and haptic technologies are also bringing down the cost of the Reachin Display environment, which is affordable to the majority of Chemistry Departments, to combine the use of haptics with 3D molecular visualizations. Initial results also indicate that our hypothesis that by using such tools, an undergraduate chemistry student will more quickly learn and understand key concepts such as molecular dynamics is correct. However, further work is needed to verify this claim by testing the use of MV in the forthcoming academic year.

### References


OpenMOIV. Open Molecular Inventor web site: http://www.tecn.upf.es/openMOIV/relatedlibs/moiv.html


Reachin Technologies, Reachin Display web site: http://www.reachin.se/products/reachindisplay/

Appendix: Calculation of the Inertia Tensor

Classically, a body rotating about an axis through its centre of mass with angular velocity \( \omega = (\omega_x, \omega_y, \omega_z) \) has rotational kinetic energy, \( T \), given by the quadratic form:

\[
T = \frac{1}{2} \omega^T I \omega = \frac{1}{2} \begin{pmatrix} \omega_x & \omega_y & \omega_z \end{pmatrix} \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix} \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}
\]

(A1)

in which the symmetric matrix, \( I \), is the (tensor of) inertia tensor. For a non-uniform body, such as a molecule, which can be described by a series of point masses, \( m_i \), representing the atom nuclei situated at \((x_i, y_i, z_i)\), the molecular centre of mass \((\bar{x}, \bar{y}, \bar{z})\) can be expressed by:

\[
\bar{x} = \frac{\sum m_i x_i}{\sum m_i} \quad \bar{y} = \frac{\sum m_i y_i}{\sum m_i} \quad \bar{z} = \frac{\sum m_i z_i}{\sum m_i}
\]

(A2)

and the moments of inertia relative to centre of mass with respect to the coordinate axes, \( I_{xx}, I_{yy} \) and \( I_{zz} \), can be expressed as:

\[
I_{xx} = \sum m_i (\beta_i^2 + \gamma_i^2)
\]

\[
I_{yy} = \sum m_i (\alpha_i^2 + \gamma_i^2)
\]

\[
I_{zz} = \sum m_i (\alpha_i^2 + \beta_i^2)
\]

(A3)

where \( \alpha_i, \beta_i, \gamma_i \) are the coordinates of atom \( i \) \((x_i, y_i, z_i)\) relative to the molecular centre of mass \((\bar{x}, \bar{y}, \bar{z})\):

\[
\alpha_i = x_i - \bar{x} \quad \beta_i = y_i - \bar{y} \quad \gamma_i = z_i - \bar{z}
\]

(A4)

The products of inertia, \( I_{xy}, I_{yz}, I_{zx} \), deviation moments with respect to the coordinate axes, can also be expressed as:

\[
I_{xy} = -\sum m_i \alpha_i \beta_i, \quad I_{yz} = -\sum m_i \alpha_i \gamma_i, \quad I_{zx} = -\sum m_i \beta_i \gamma_i
\]

(A5)

The coordinate axes \((\alpha, \beta, \gamma)\) can be rotated to coincidence with the principal axes \((\alpha', \beta', \gamma')\) for that body, resulting in the inertia tensor becoming diagonal, and the rotational kinetic energy, \( T \), for the molecule rotating about its centre of mass within that principal coordinate frame becomes:

\[
T = \frac{1}{2} \begin{pmatrix} \omega_x & \omega_y & \omega_z \end{pmatrix} \begin{pmatrix} I_{xx} & 0 & 0 \\ 0 & I_{yy} & 0 \\ 0 & 0 & I_{zz} \end{pmatrix} \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}
\]

(A6)

and is only comprised from rotational contributions about the principal \( \alpha', \beta', \gamma' \) axes.

Similarly, the angular momentum for a rotating body, \( \mathbf{l} \), is related to its angular velocity, \( \omega \), by:

\[
\mathbf{l} = \mathbf{I} \omega = \begin{pmatrix} l_x \\ l_y \\ l_z \end{pmatrix} = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix} \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}
\]

(A7)

Diagonalisation of the inertia tensor, \( \mathbf{I} \), only occurs when the coordinate axes coincide with the principal axes of inertia, reducing Equation 4 to:

\[
l_x = J_x = I_{xx} \omega_x \quad l_y = J_y = I_{yy} \omega_y \quad l_z = J_z = I_{zz} \omega_z
\]

(A8)

and the kinetic energy, \( T \), becomes:

\[
T = \frac{l_x^2}{2I_{xx}} + \frac{l_y^2}{2I_{yy}} + \frac{l_z^2}{2I_{zz}} = \frac{J_x^2}{2I_{xx}} + \frac{J_y^2}{2I_{yy}} + \frac{J_z^2}{2I_{zz}}
\]

(A9)

The eigenvalues and corresponding eigenvectors are sorted so that \( I_x \leq I_y \leq I_z \), and the principal coordinate frame for the molecule is rotated so that \( I_x \) aligns with the \( x \)-axis, \( I_y \) aligns with the \( y \)-axis, and \( I_z \) aligns with the \( z \)-axis. This is one of six possible orderings encountered within Molecular Spectroscopy.