

A 3D Molecular design and Management using Data Glove Interaction Technique

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Abstract: *The creation of meaningful knowledge in Molecular world has been the great challenge in chemistry learning process. This paper proposed an interactive 3D design of Molecule and develops an alternative input device for interacting with it for molecules manipulation. This article describes the steps on the development of low cost data glove based on Contact switching technique. Also it shows a set of preliminary result obtain in Molecular application with the input Data Glove and discuss the use of Molecular application that could be supportive and helpful for student in chemistry learning process. The result shows that Data glove interaction is more accurate and natural than keyboard and mouse in operating 3D Molecular environment. It also enhances the user interaction in Chemistry studies and feels immersion in using Human Computer Interaction (HCI) technique.*

Keywords: Contact Switch, Data Glove, Arduino Microprocessor, 3D Molecular Dynamics, Virtual Reality, Visualization.

1. Introduction

Technological revolution has made an enormous positive effect in the field of science and technology. In addition, it has provided an engineering solution to human computer interaction in building virtual application. Human's have many more capabilities of balancing the sense and whatever we know about our reality come through the way of our sense. Our perception of reality would also be change in response that present with version of reality that isn't really there, is refers as virtual reality. The present work discusses the use of virtual Molecular application that helps student of chemistry to deals with the original studies reasoning in science. The basic use to obtain such application is to understand the basic structure of molecule [1] [2].

Traditionally, the science studies were done using physical models such as balls and sticks, Microscope and many more ways. Those models become very difficult to understand in grasping the real molecular structure for learners [3]. Students creates many misconception while using microscope for chemistry teaching (Example: atoms, bonds, molecules, structure) [4] [3]. The problems such as:

- Choosing the central atom, completing its bonding, drawing the Lewis structure difficulties that learners posses [5].
- Analyzing the real structure of Molecule
- The balls and sticks models are rigid, and students commonly face difficulties in comparing the difference in bond angle, size, weight, length, etc. of different molecule. Thus they lack in representing adequately.

Therefore, the idea of the paper is to developed an appropriate learning and teaching tools using VB.NET application that

helps learners to improve their imagination in the world of science that conceptually understand effectively. The present works designs an interactive design of molecules in 3D and provide the possibility of visualization.

Virtual reality system [7] is aimed at molecule of hand movements using Contact Switching technique depend on input

devices to capture the data associated with finger pressing. As discuss previous Data glove are commonly used in virtual reality system. According to Jadon and Murthy [10], basically there are two main approaches to capture hand gesture: the computer vision technique or Data Glove technique.

Data Glove using Contact Switching technique [8] is an intermediary device constrains the interaction with the application. There are many options available commercially such as CyberGlove (www.cyberglovesystem.com), the 5DT Data Glove (www.5dt.com), and NED Glove (acronym for NeuroEnigo Design) [9]. The motivation for developing those gloves was stemmed from the need to create a low cost Data Glove. The present Data glove is simply developed using Contact Lever Switch [12] and build on the properties of switching technique to allow a visual feedback. We developed a set of Molecular application to allow the feedback from the glove inputs, describe in section 3.

2. Background

Many challenges and research presents the interactive system that makes a practical world more realistic in the field of science. In a traditional classroom, molecular geometry was taught by lecturing; by using chalk and blackboard as discuss [4]. The utilization of innovative and emerging technologies in education provides new learning environments that supports, authentic, meaningful, realistic experiences (Barab et al, 2007; Squire and Jan et al 2007).

Georgiou et al 2007, recognized a significance advance that Provides an opportunities and learning experiences for students with microscopic molecular structures in 3D simulation. Muhanna [4] states that user's actions are sensed in virtual environment in which the participants can have the feeling of being mentally immersed. The instructors can create virtual learning environment in which students can able to interact with real-like objects related to scientific concepts (Bricken, 1990). Dendral program [11] made by Edward, Bruce and Carl is considered as the first expert system in automatic decision making process and problem solving behavior of organic chemistry (Carbon atom).

CAVE [13] was explicatively design for scientific visualization to explore how molecules interact. It produces a sense of immersion by surrounding a user with wrap-around-screen through the images projected in stereo on the walls. The CAVE was first applied to drug treatments called “Chagas” dieses.

Human Computer interaction (HCI) allows alternative input devices for interacting with computer in virtual application replacing with standard keyboard and mice [15] [14]. The visual feedback is being usually developed and implemented with 3D virtual hand. Some of the implementation uses OpenGL to design the VR hand simulator. Many work also proposed a unity to create a simulator for emergency medical training. Kumar [17] proposes a system that can captured data with a Data Glove to manipulate a virtual objects. Kumar also used the VHand V2.0 to develop a system that interprets hand gesture related a click and point a movements usually made with a mouse.

The work of Connoly [22] developed a 5DT 14 Ultra Data Glove for an application that capture the movements from each finger and are displayed in realtime in numerical and graphical form that uses accurate angle measurement of digits in human hands.

3. Methodology

The project contributes of two major parts: Data Glove implementation and development of 3D Molecular application virtually. Figure 1 is the block diagram of hardware and software interface that shows the communication channel between microcontroller and processing through USB.

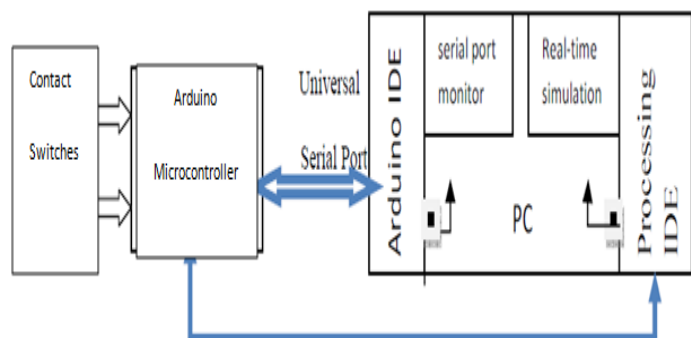


Figure 1. Hardware and Software interface

3.1 Data Glove Design and implementation

The Data Glove is implemented using five Contact Switches. Figure 2 illustrate the signal conversion circuit for Glove input. The circuit composed of a set of five Contact Switches, the interfacing unit and Arduino Uno microcontroller and an USB cable connecting microprocessor to PC.

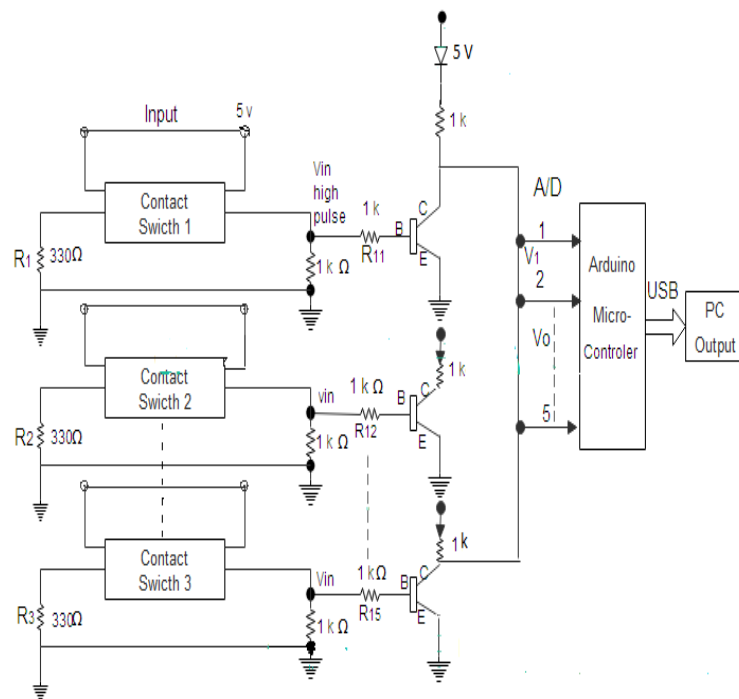


Figure 2. Signal Conversion Circuit (convert resistance to voltage)

Initially, the working shows that, as per the user requirement user will press the switches for the virtual appearance (Note each finger is assigned with switch and each switching properties contain different operations to be perform). The analog outputs from the switch are supplied to the microcontroller via serial interface. So, when user will shuffle the finger on switch, the binary digit will get generated as shown in Figure 3.



Figure 3. Serial port output obtain

The VB.Net program with switch case algorithm will compare the digital signal into a digital sequence as shown in Figure 3. The microcontroller is connected to PC via a USB port for serial communication. The Arduino IDE based on C programming is used to program the microcontroller. Arduino IDE has a serial port monitor that monitor the real-time response of hardware in numerical values. The virtual 3D hand Data Glove is implemented in processing IDE which is another C based programming environment. And using this serial communication commands in processing, a serial communication channel (SSC) get established between microcontrollers connected to the switches. Figure 1 shows the

communication between PC and microcontroller. The circuit shown in Figure 2 has transferred the function of:-

$$V_o = \left[\frac{R_1}{R_{11}} V_{in} + \frac{R_2}{R_{12}} + \dots + \frac{R_5}{R_{15}} V_{in} \right]$$

Whereas, V_{in} is the buffer output produced by the switching activity and V_o is the final output of overall circuit. The circuit adds positive voltage value to the buffer circuit so that the low negative voltage is offset by the comparably higher voltage of the circuit output. Finally, small voltage generated and gives amplified voltage that falls within the desired voltage range. Beside the circuit topology, the data actuation algorithm for Microcontroller is adapted illustrated in Figure 4.

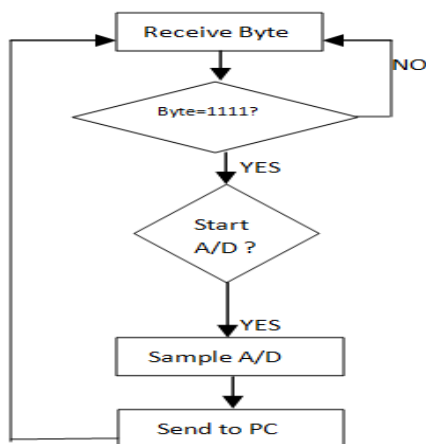


Figure 4. Data Acquisition Algorithm

The flow indicates that on receiving the input, a decision has to be made to check if the received byte is of certain value or range. The signal received shown in Figure 3 while Data Glove is connected at port "COM7".

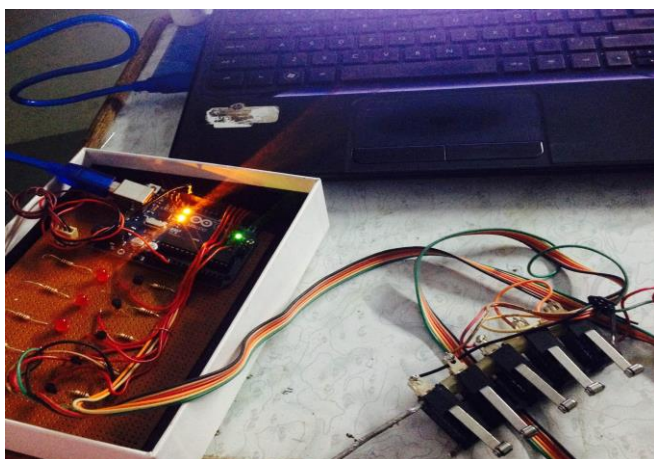


Figure 5. Finalized working circuit

3.2 3D Molecular Design and Development

Molecules are in 3D but visualization is difficult. To simulate those basic structure of molecules, the atom and the behavior of atom must be understand [1][2][16]. The primary tool used for computing and development of molecules in 3D visualization is VB.Net application. So as discuss previous (section 1) that once the digital sequence match for the corresponding motions or movement of 3D image, the function of 3D image will be called. This process will be repeated for multiple motions as per the user requirements. It is capable to translate five

operations on the displayed molecules. Generating the molecules is the complex calculation. The backend Microsoft office is used as 3D engine that act as database system which stores the information or properties of molecule. Paper [18] states and describes the algorithm used to generate molecules and calculating the dimension for displaying atoms and their bonding in Sphere and Cylindrical form as below:

- Assigning Atoms with number of Sphere (SPH) and Cylinder (RSPH) by formula:

$$\begin{aligned} \text{Atom}(\text{AtomInd}).\text{Sph1}(i, \theta) &= \text{cir} \\ \text{Atom}(\text{AtomInd}).\text{RSPH1}(i, \theta) &= \text{cir} \end{aligned}$$

$$\begin{aligned} \text{Atom}(\text{AtomInd}).\text{Sph1}(i, 1) &= r * \text{Math.Cos}((\text{theta} * 3.14) / 180) * \\ &\quad \text{Math.Sin}((\text{fia} * 3.14) / 180) + \text{CenterX}/y/z \end{aligned}$$

-Bonding development with:

$$\text{Bond}(\text{BondInd}).\text{Cylinder}(i, \theta) = p * \text{Math.Sin}((\text{theta} * 3.14) / 180) + \text{CenterX} \text{ 'x/y/z}$$

-Calculating ANF, SINVAL AND COSVAL by formula:

$$\begin{aligned} \text{Ang} &= (4 * 3.14) / 180 \\ \text{SinVal} &= \text{Math.Sin}(\text{Ang}) \\ \text{CosVal} &= \text{Math.Cos}(\text{Ang}) \end{aligned}$$

-Assigning rotation to Sphere and Cylinder by formula as:

$$\begin{aligned} Z1 &= \text{Atom}(\text{AtomInd}).\text{RSph2}(i, 3) * \text{CosVal} - \text{Atom}(\text{AtomInd}).\text{RSph2}(i, 1) * \text{SinVal} \\ X1 &= \text{Atom}(\text{AtomInd}).\text{RSph2}(i, 3) * \text{SinVal} + \text{Atom}(\text{AtomInd}).\text{RSph2}(i, 1) * \text{CosVal} \\ \text{Atom}(\text{AtomInd}).\text{RSph2}(i, 1) &= X1 \end{aligned}$$

$$\begin{aligned} Z1 &= \text{Bond}(\text{BondInd}).\text{Cylinder}(i, 2) * \text{CosVal} - \text{Bond}(\text{BondInd}).\text{Cylinder}(i, \theta) * \text{SinVal} \\ X1 &= \text{Bond}(\text{BondInd}).\text{Cylinder}(i, 2) * \text{SinVal} + \text{Bond}(\text{BondInd}).\text{Cylinder}(i, \theta) * \text{CosVal} \\ \text{Bond}(\text{BondInd}).\text{RCylinder}(i, \theta) &= X1 \\ \text{Bond}(\text{BondInd}).\text{RCylinder}(i, 1) &= \text{Bond}(\text{BondInd}).\text{Cylinder}(i, 1) \\ \text{Bond}(\text{BondInd}).\text{RCylinder}(i, 2) &= Z1 \end{aligned}$$

The 3D engine allows: retrieving the particular molecule that is created by adding values as per the atoms and bonding properties by the user itself. After retrieving, it is being displayed with standard dimensions. Figure 6 shows the snapshots of database.

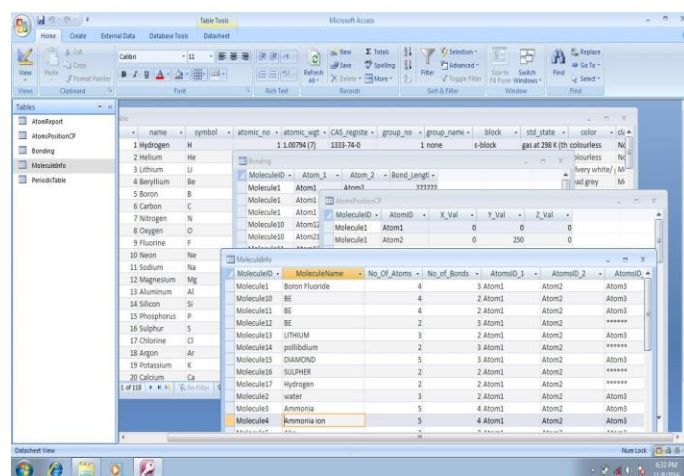


Figure 6. Database snapshots

The 3D engine contain all the information and chemical properties of molecules like symbol, atomic weight, atomic number, bond angle, Bonding Radius, center co-ordinates for atom in molecule.

4. Experiments and Results

The experiments shows the wired Data Glove developed with Contact Switches, Arduino Microprocessor as discuss in previous section. Arduino processing IDE as shown in Figure 1 is 'C' based programmable environment for developing animation, simulation, real time interaction. The signal from Data Gloves is send to analog inputs pins on the microcontroller for bridging the connection between the hardware and PC. An appropriate program is written and uploaded on Arduino to setup a serial port communication channel between microcontroller and signal conversion circuit. Figure 3. Shows the signals connection received from the Data glove inputs.

Table 1. DataGlove Position

SR.NO	X Rotation	Y Rotation	Z Rotation	Arbitrary Rotation	Comments
1.	0	0	0	1	Arbitrary = High, Perform Arbitrary Rotation
2.	0	0	1	0	Z = High, Perform Z axis rotation
3.	0	1	0	0	Y = High, Perform Y axis rotation
4.	1	0	0	0	X = High, Perform x axis rotation

Data Glove position on the PC matching the blocks compares the input signals. Table1. Shows Data glove position for different operations. Than the application gets the word to be processed treats the word and takes decision by setting the corresponding bits on serial port when those corresponding LED well get on.

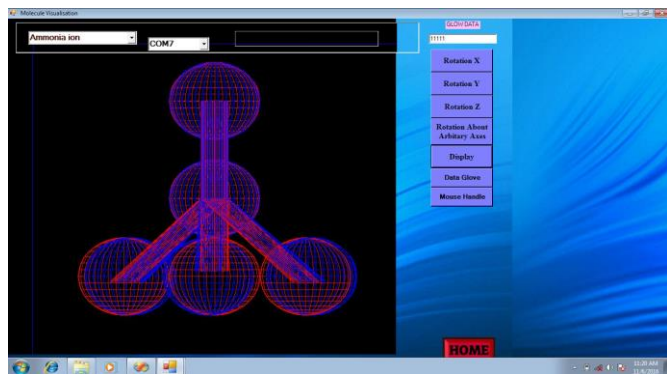


Figure 7. The GUI output Screen of the program

Figure 7 shows molecule selection and operational commands. Within virtual environment, on the particular selection, the screen will display with Ammonia ion molecule. It shows the initial state of the molecule. The final outputs for different operations are as:

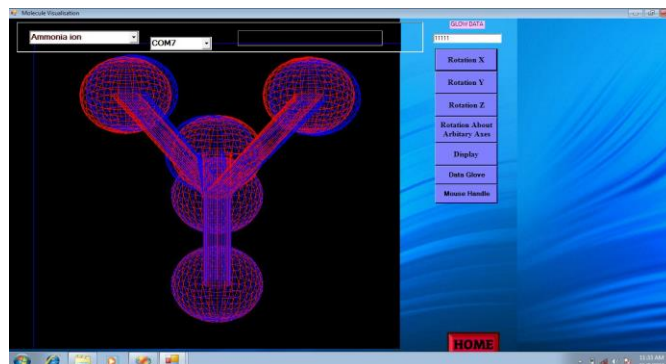


Figure 8. Result of Data Glove input for X-rotation

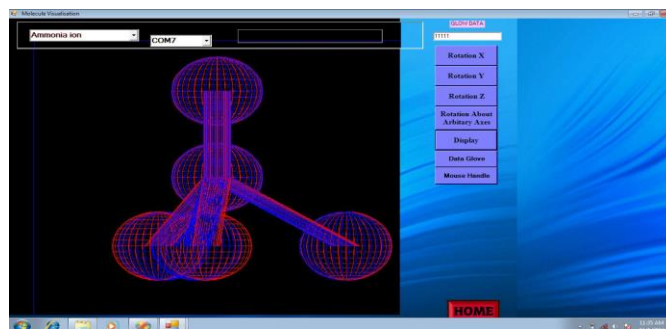


Figure 9. Result of Data Glove Input for Y-rotation

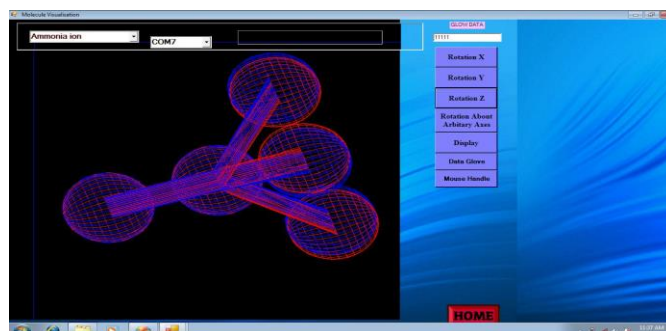


Figure 10. Result of Data Glove Input for Z-rotation

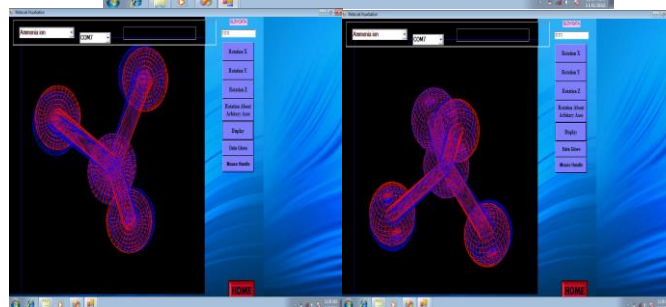
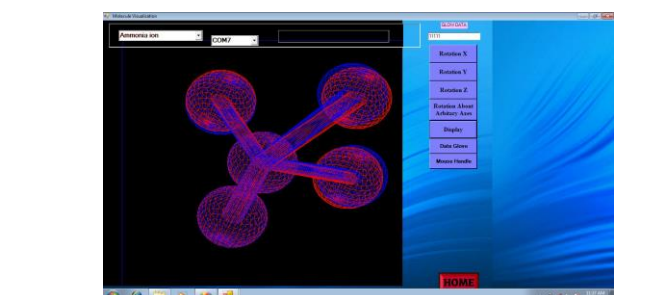


Figure11. Result of Data Glove Input for Arbitrary –rotation

5. Conclusion and Future work

Due to the limitation and increasing misconception in the field of chemistry learning process, it was necessary to devise a

computer –aided molecular design to visualize the reality. The aim of the project is to determine the learner molecular knowledge prior to the way of teaching and enhance learner’s conceptual understanding. The present work describes a system that build molecule in 3D visualization. The use of computer-based molecular simulation tools is successfully running for four operation of rotation with an interface based on Data-Glove technique that can be implemented with relatively simplicity using Contact Switch. It is integrated with virtual reality object to assist with the objects. The Data Glove is capable to do rotation on 180° degree of freedom for each operation. The proposed work is done with wired Data Glove that is hard to carry and complicated with multiple users. In future the project can be extended with wireless Data Glove, so that it well also made possible to manipulate molecule in different forms and thus it will easily rotated through Data Glove.

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