A 3D Atomic Bonds Rendering with DataGlove for Creating Virtual Environment

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***Abstract*—Virtual Reality is one of the most important real-time aspects in today's world. The proposed work is to develop a virtual world for exploring the interaction of atomic bonds. In traditional system molecules increase in complexity. Physical model become very cumbersome to assemble and the geometric structure of the atoms can be difficult to interpret. Due to limitations in physical nature and increased speed and availability of computers, computer simulation tools can be used to create improved molecular models for learning. The proposed approach is to develop a low cost wireless Dataglove that can implemented with relatively simplicity. It can be integrated with virtual reality for 3D atomic bonding structure. The idea is to design two aspects i.e. developing a low cost Dataglove and to design a simple, expandable computer modeling program for different molecular structure. The aim of the project is to aid in the understanding of molecular structure and interaction in a way that is realistic and enjoyable to user.**

***Keywords*—Virtual Reality, Wireless IRTxRx DataGlove, Atomic bonds, Arduino Microprocessor, Movement for finger.**

I. INTRODUCTION

Students experience a number of problems during the learning process of students like molecular biology, particularly when students study molecular structure [3]. When molecules increase in complexity [1], physical models become very difficult to understand and the geometric structure of the models is difficult to interpret. Their comes difficulties to comprehend 3D structure of atoms that build up a molecule [2], the way molecules bond to each other and so on. Particularly, the use of plastic and wooden molecular model was used to assemble the actual structure of bonds. Thus, these models present some limitations, since they are insufficient to show certain characteristics of an atomic bonds structure [2]. Therefore, there is enough information to understand the physical nature of the molecule and difficulties to gain the understanding [13].

The proposed system is a real time application of learning molecular structure in 3D view [4]. Virtual Reality is a computer generated space [3] in three dimensions (called as virtual environment) that is highly interactive. The virtual appearance is applied to atomic bonds. The program is to render the human interface for interaction with atoms and build molecules in 3D virtual world.

The Data glove [7], [11] technique is design to captures finger articulation, hand motion and orientation [5], that grasped the data for the gesture interaction in the human-computer interface [5], [6]. These gloves carry a set of sensors that capture information related to object grabbed by the hand [7].

Most commonly and marketed hand-tracking gloves [6] include MIT LED glove, Digital Data Entry Glove, Cyber Glove, Power Glove, Dexterous Hand master, Sayre Glove and Space Glove [8], [11]. There are several types of sensing technologies that have been applied to the development of Dataglove. And most of these provide high accuracy, high capability, and reliability in measuring the Degree of Freedom (DoF) of human hands [15], [20], [11]. Therefore most of them are constructed using sensors that measure the bending angels of fingers.

But these commercial gloves usually uses are expensive motion sensing fibers and motion analyzers, and are too costly. Therefore, one of the most important scopes of the project is to design the low cost wireless Data glove called as Wireless IRTxRx Dataglove. This glove is home-made version of Dataglove.

It consists of IR transmitter and Receiver. The effort facilite the easy availability of microcontroller chip known as Arduino microprocessor [12], [20] which is described in section III. The present work is to:

1) Create Virtual environment for the atomic bonds (e.g. water, ammonia, oxygen and many more) using VB .Net application.
2) Implementing wireless IRTxRx dataglove for motion capturing.
3) Hand-motion and orientation tracker and interfacing it with 3D image of atomic bond structure, making the movements of atoms.

II. RELATED WORK

The Previous researches have shown the development of NED dataglove to control the video game application rehabilitation of stroke patients by Lucas Silva and Andre [7]. The experiments show the new rehabilitation programs that can help patients to regain independence in daily live activities. This NED

glove which was the advantage over the four glove based system as shown in table 1. He designs a glove which contains IMU, Viber Sensor. The language used was JavaScript and C#, where physical simulation was possible.

The finger movements and hand gesture is usually implemented with a virtual 3D hand. Some implementation use openGL [13], to design the virtual hand simulator in order to interact. Nazrul H [14] developed a "GLOVEMAP" [14], in which the minimum and maximum data of the fingers movement between thumb, index and middle finger using the Principal Component Analysis (PCA) is done.

Connoly [9] developed an intelligent computing to assist clinicians using data glove 5DT 14 ultra. He uses accurate angle measurement of digits in the human hand with a data glove. Paper [15] discusses the design consideration for a wearable monitor to measure finger posture. The author design an analysis of a wearable sensor glove specific with a specific focus on the sensors selected to measure bend. It introduced the sensor selection and glove evaluation process. The previous evaluations for bend sensors the repeatable measurement of finger flexion which was not appropriate. Therefore, the case study for sensor glove [15] was design which shows high degree of repeatability.

Table 1 shows the comparison between existing and proposed DataGlove technique.

Project	Data Glove	Sensors	Language	Physical Simulation
Connoly et. [22]	5DT dataglove 14 ultra/X-IST dataglove HRI	Accelerometer	Not Mention	No
Zhu et. [21]	5DT dataglove	Accelerometer	Visual C++	No
Kumar et. [22]	VHand DG5 V2.0	Accelerometer	C++/C	No
Teleb et. [24]	VHand DG5 V2.0	Accelerometer	C++	Yes
Lucas silva [7]	NED Glove	IMU,Viber	JavaScript	Yes
Wireless IR TxRx Dataglove	IR TxRx Glove	IRTxRx	VB.net and C#	Yes

Table 1. Comparison

The traditional lectures to the student may be difficult to grasp the scientific concept of molecular science [1], [2]. Sankaranarayanan integrated visual, haptic, and auditory stimuli in implementation of simulation in which voice commands are used to manipulate and obtain feedback on 3D molecule [18].

Trindade and Fiolhais [16] developed the complex 3D graphics to render a virtual environment of water molecules using the Cyber glove and head mounted display. In using virtual environment for studying water phase and phase transitions by Jorge F [10], creates a Cyber touch system associated to the data glove which enables the user experience for molecular behaviour that is impossible to feel in the real world. The interaction of this Cyber glove allow the user to act and change the environment in order to distinguish the properties of solid, liquid, and gases. The experiment shows the balls model of a group of molecules flying through the ice structure.

By examining past efforts, I proposed a easy setup and simple simulation program to make the virtual environment for bonds and apply the IRtxRx Dataglove technique which is enjoyable to user.

III. SYSTEM DESIGN

The Project contributes two major parts: i.e. Dataglove implementation and simulation of virtual environment for creating atomic bonds structure.

A. IR TxRx Dataglove

The dataglove is assembled with a five pieces of IRTxRx sensors which will be attached on the finger joint positions of the hand. Also the named is given as Figure 1 shows the proposed system architecture.

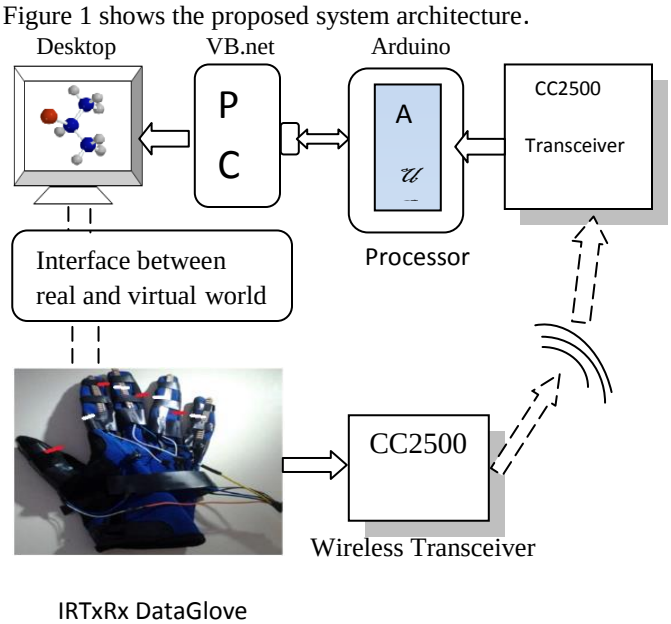

Figure 1. System Architecture

IRTxRx Dataglove because all the movement of the fingers is based on the five pairs of IR Transmitter and Receiver placed on finger of the glove. Figure 2 shows

block diagram of the hardware part of the project to the PC setup for Virtual interaction.

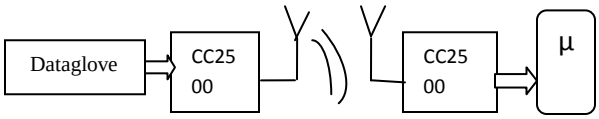

Figure 2.Hardware simulation

The steps given below shows the working of dataglove:

- As per the user requirement user will insert the finger for the virtual appearance.
- When the finger inserted in between IR transmitter and Receiver, the output of transistor (BC547) is high else it is low.
- So, when user will shuffle the finger in the glove, the binary digit will get generated.
- Than that Binary digit will get directly serially generated on wireless transreciver (CC2500).
- And simultaneously CC2500 will receive the binary digit.
- A VB .Net programme with switch case algorithm will compare that digital signal into a digital sequence using switch case algorithm.
- Once the digital sequence is match for that corresponding motion or movement of 3D image, that function of 3D image will be called.
- This process will be repeated for multiple motions as per the user desertion.

B. A Simulation for Atomic Bond

Molecules are in 3D but visualization is difficult. To simulate basic molecular interactions, the atoms and behaviour of atoms must be understood [1], [2], [3], [4]. My simulation program is restricted to single bonds, but it can be further to double and triple bonds. In the present simulation, the similar atoms like hydrogen, ammonia, water, oxygen, carbon are used. The values for length and energies of bond depend on factors like atom size, atom structure, electro-negativity and electrons affinities. They are described and stated in plots [19]. Therefore this requires complex calculation. The primary advantages are that the molecule can be built quickly, represented according to the user's preferences, and manipulated easily. This function provide the zoom facility such as zoom in, zoom out, panning and rotation about axes. Algorithm 1 shows pseudo code for generating atomic bond structure.

There are three sub-modules:

1. 3D Engine: It contain the information, properties of molecules like symbol, atoms weight, atom number, bond angle, bonding radius, centre co-ordinates for atoms and so on.

2. Stereoscopic vision: Mainly visualization of molecule is difficult. In a stereographic 3D image, you can actually see the depth. For identifying the image, the two different filters are used red/green to view image. The molecular modelling is done with balls and stick, spiral and capsule.

3. Navigation: It manipulates the molecule using the Data glove. As discuss in part [B] for navigation wireless IRTxRx Dataglove is used. The figure 3 shows the general flow of the project.

Algorithm 1:

```
1) First open the database
2) Read Molecule Name"Molecules", "No of atom", "No of bonds. From Table.
3) Then Calculate the CenterX, CenterY, CenterZ for bonds display.
4) For step 3 open the database connection and read rows at index of J (for e.g.) for X,Y,Z Value.
5) For J=0 to Atoms Position with its Row Count if Moleculeid=AtomsPositionCPDT.Rows  then go to next step
   below.
6) Then for Loop Of FIA -90 to 90 degree with step 10 increment and within for loop
7) Theta for -180 to 180 degree increase with step of 10 assign atom with number of SPH and RSPH with formula
   given below:
        Atom (AtomInd).Sph1 (i, 0) = cir
        Atom (AtomInd).RSph1 (i, 0) = cir
        Atom (AtomInd).Sph1 (i, 1) = r * Math.Cos((theta * 3.14) / 180) * Math.Sin((fia * 3.14) / 180) +
   CenterX
        Atom (AtomInd).Sph1 (i, 2) = r * Math.Sin((theta * 3.14) / 180) + CenterY
        Atom (AtomInd).Sph1 (i, 3) = r * Math.Cos((theta * 3.14) / 180) * Math.Cos((fia * 3.14) / 180) +
   CenterZ
        Atom (AtomInd).RSph1 (i, 1) = r * Math.Cos((theta * 3.14) / 180) * Math.Sin((fia * 3.14) / 180) +
   CenterX
        Atom (AtomInd).RSph1 (i, 2) = r * Math.Sin((theta * 3.14) / 180) + CenterY
        Atom (AtomInd).RSph1 (i, 3) = r * Math.Cos((theta * 3.14) / 180) * Math.Cos((fia * 3.14) / 180) +
   CenterZ
8) For number of Rows Count increment AtomIND and CIR by 1
9) Repeat 6 & 7 step for another sphere.
10) Now we go for bonding development next by reading molecule and again Center X, Y, Z.
11) Then for theta = 0 To 360 Step 10
        Bond (BondInd).Cylinder (i, 0) = p * Math.Sin ((theta * 3.14) / 180) + +CenterX "x
        Bond (BondInd).Cylinder (i, 1) = CenterY "y
        Bond (BondInd).Cylinder (i, 2) = p * Math.Cos ((theta * 3.14) / 180) + +CenterZ "z
        i = i + 1
    Next
12) Increment Bondid by +1
13) Then calculate ANF, SINVAL AND COSVAL by formula
        Ang = (4 * 3.14) / 180
        SinVal = Math.Sin(Ang)
        CosVal = Math.Cos(Ang)
```

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14) Now Assign rotation to sphere and cylinder cylinder by formulas as below:
        For AtomInd = 0 to No_of_atom - 1
        For i = 0 to Npoint - 1
            Z1 = Atom (AtomInd).RSph1(i, 3) * CosVal - Atom (AtomInd).RSph1(i, 1) * SinVal
            X1 = Atom (AtomInd).RSph1(i, 3) * SinVal + Atom (AtomInd).RSph1(i, 1) * CosVal
            Atom (AtomInd).RSph1(i, 1) = X1
            Atom (AtomInd).RSph1(i, 3) = Z1
          Next
        Next
        For AtomInd = 0 to No_of_atom - 1
          For i = 0 to Dpoint - 1
            Z1 = Atom (AtomInd).RSph2(i, 3) * CosVal - Atom (AtomInd).RSph2(i, 1) * SinVal
            X1 = Atom (AtomInd).RSph2(i, 3) * SinVal + Atom (AtomInd).RSph2(i, 1) * CosVal
            Atom (AtomInd).RSph2(i, 1) = X1
            Atom (AtomInd).RSph2(i, 3) = Z1
          Next
        Next
        For BondInd = 0 To No_of_bonds - 1
          For i = 0 to NoIndexCylinder - 1
            Z1 = Bond (BondInd).Cylinder (i, 2) * CosVal - Bond (BondInd).Cylinder (i, 0) * SinVal
            X1 = Bond (BondInd).Cylinder (i, 2) * SinVal + Bond (BondInd).Cylinder (i, 0) * CosVa
            Bond(BondInd).RCylinder(i, 0) = X1
            Bond(BondInd).RCylinder(i, 1) = Bond(BondInd).Cylinder(i, 1)
            Bond(BondInd).RCylinder(i, 2) = Z1
          Next
        Next
15) Finally closed the connection by PEN properties
        MyBpen = New Pen(Color.Blue, 1)
        MyRpen = New Pen(Color.Red, 1)
16) Display_Molecule with MYBPEN and MYRPEN
17) Thus bond is displayed and we can add Dataglove Function after also...
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C. Arduino Microcontroller

In this project, Arduino processor are used for hardware and software interface, because it is easily available in market which is less in cost. Arduino microprocessor [12], [17] is the communication system that functions as a sense to the environment by receiving the input from the dataglove. It involves the design of objects that can communicate with humans using sensors and actuators [12]. It is controlled by a behavior implemented as software running inside a small computer on a single chip.

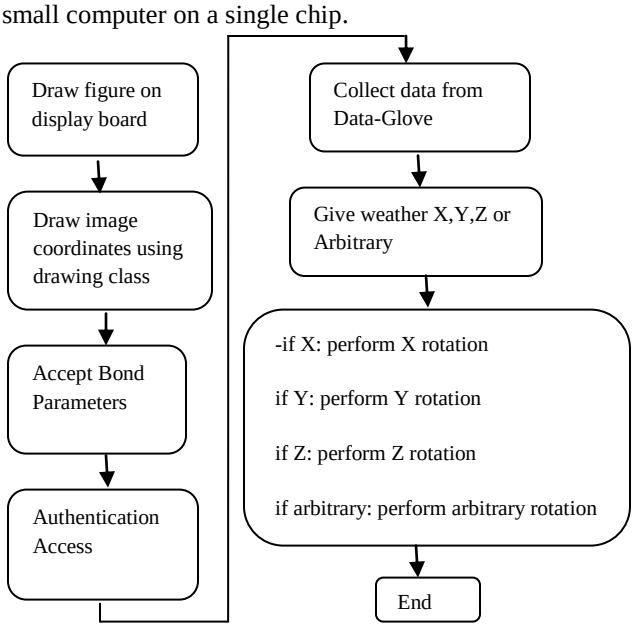

Figure 3. Flow Diagram

IV. COMPARISION

Rotation of the Bond could be adjustable as per user hand movement. And for interruption of finger in IR pair, will produced 10° rotations. There is no actual physical motion of sensor. So there is no wear and tear of sensor glove. Therefore the glove can sustain for lifelong.

CONCLUSION

The objective of the project is to develop a low cost Dataglove technique in order to enable the molecular model that make the user to feel the electrostatic forces between atoms and group of atoms with 3D virtual views. The approach is to design a simple, expandable computer modeling program and enhance it with virtual environment. This application is design for educated users and can be used in chemistry study, multimedia, pharmaceutical study, molecular bio-science and so on. Hence, the experiment shows that the simulation environment could be expanded to atomic bonding. The IRTxRx Dataglove is capable to improve the finger movement as compared to existing.

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