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Virtual Environment for Exploring Atomic Bonding

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Abstract. A virtual world for exploring the interactions of atoms is described. The program was created in order to provide an alternative to traditional methods of teaching chemistry to pre-college students. A haptic interface allows a user of the program to experience a recreation of the forces that would be present during real world atomic interactions. A first order simulation of atomic interaction is described, sufficiently simple that real-time calculations may be performed with the model. The program underwent preliminary testing during a hands-on demonstration. Based on initial feedback from users, an experiment was designed to evaluate the benefits of haptic feedback in assembling molecules. The results show that by providing force feedback, it is possible to decrease the amount of time required to create a simple molecule in a virtual environment. The next phase of testing will be to demonstrate the utility of the simulator in an elementary school classroom.

1 Introduction

It can be challenging to teach students the underlying principles of molecular biology and chemistry due to the microscopic scale of the subject matter. For years, physical models, such as ball-and-stick and van der Waals spherical models, have been used to help students gain intuition for the spatial relationships of molecules and their inherent flexibility. While these can be good tools for geometric representation, they fail to provide the student with a good understanding of the forces and interactions between the atoms and molecules involved in atomic bonding. Additionally, when molecules increase in complexity, physical models become very cumbersome to assemble and the geometric structure of the models can be difficult to interpret. Due to the limitations of physical models and the increased speed and availability of computers, computer simulation tools can be used to create improved molecular models for learning.

Using computer graphics programs to explore molecules has become a ubiquitous tool for research scientists in experimental and computational biology. Commercial molecular modeling packages include: Rasmol, Protein Explorer, Pymol, Insight, and Swiss PDB Viewer. The primary advantages of computer modeling programs are that the molecule can be built quickly, represented according to the user's preferences, and manipulated easily. Atoms can be rendered in a variety of colors and

shapes to portray different functional regions, and movies can show functional motion of the molecule. However, these tools are designed for educated users. The user does not gain any physical intuition into the necessary forces required for the structural development and changes in the molecule. While this may be enough information for an educated research scientist to understand the physical nature of the molecule, it may be difficult for a novice student to gain the same understanding. Therefore, we created a program for the beginning user designed to teach the fundamentals of atoms and molecules. Our approach was to design a simple, expandable computer-modeling program and enhance it with haptic feedback. Using haptics in the molecular model enables the user to feel the electrostatic forces between atoms and groups of atoms. Key information presented includes the strength of molecular bonding, properties of full and partially full valance shells in bonding, and an understanding of how these properties affect the geometric structure of the molecule.

A program has been developed that allows a PHANTOM haptic device [1] to be used for interaction with atoms and build molecules in a 3-D virtual world populated by hydrogen, carbon, and oxygen atoms. The program can be expanded to accommodate any number of atoms, atom types, and atom properties, allowing each designer to personalize the simulation to best meet his or her individual teaching needs. Our goal is to provide a general tool to aid in the understanding of molecular structure and interactions in a way that is realistic and enjoyable to the user.

2 Background

2.1 Using Graphics and Haptics in Learning Science

Research has shown that traditional lectures alone may not be enough to for students to grasp difficult scientific concepts [2]. If one can immerse the student in a scientific experience and create a learning-by-doing environment, the student may be able to conceptualize and retain a mental model more easily. Researchers have implemented visual, haptic, and auditory feedback in a variety of ways. Sankaranarayanan integrated visual, haptic, and auditory stimuli in a simulation in which voice commands and the hands are used to manipulate and obtain force feedback on a virtual molecule [3]. Trindade uses complex 3D graphics to render a virtual environment of water molecules using the Cyberglove and a head mounted display [4]. The GROPE project uses haptic feedback to portray force fields in molecular docking simulations [5]. Dede examined the role of using virtual reality to convey abstract scientific concepts and used the findings in three immersive worlds [2]. When designing an immersive environment, several factors should be considered: (1) The environment must be attractive and enjoyable to the user. In other words, design a tool that motivates the user to learn. (2) The model must be original, realistic, and enhance the learning process when compared to traditional approaches. (3) The model must be simple, flexible, and expandable, so that a variety of examples and concepts can be demonstrated and students at all learning levels can benefit.

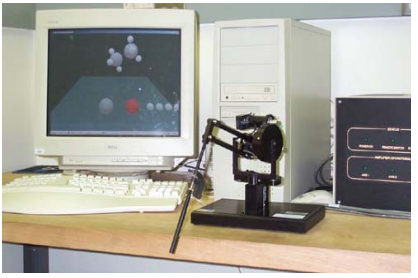

Fig. 1. An overview of the atomic bonding simulation workstation

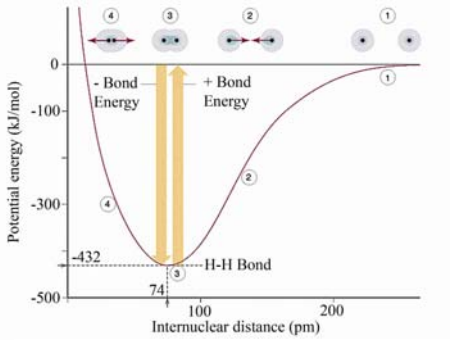

Fig. 2. Leonard Jones potential plot for Hydrogen-Hydrogen bonding [6]

By examining past efforts and the following criteria, we designed the virtual world simulation for atomic bonding. Using the PHANTOM as the haptic interface and using OpenGL graphics makes our virtual environment non-invasive and requires little setup. The easy setup and simplicity of the simulation program makes it an ideal virtual environment for a museum exhibit or school demonstrations. An overview of the system is shown in Figure 1.

2.2 A Realistic Simulation

To simulate basic molecular interactions, the atoms and the behavior of the atoms must first be understood. The bond order, bond length between two atoms, and the bond energy are a few important properties of interacting atoms. The bond order describes the number of bonds shared between the atoms, and is commonly referred to as single, double, and triple bonding. Our initial simulation program is restricted to single bonds, but could easily be extended to double and triple bonds. Bond lengths and bond energies are found in standard chemistry handbooks. For similar atoms like those used in the current simulation (hydrogen, carbon, and oxygen) the bond lengths for single bonds are the sum of the two covalent radii and range from 74pm (picometers) for hydrogen to over 250pm for larger atoms such as bromine. Thus, the covalent radii will typically increases with atomic mass. The bond energy is the bond strength or energy required to break a single bond. Typically, as the bond length decreases, the bond energy increases. The values for bond lengths and bond energies depend on many factors including atom size, atom structure, electronegativity, and electron affinities; this can require complex calculations. Therefore, they are most commonly described in plots, such as the Leonard-Jones potential shown in Figure 2 [6].

Using a model of the forces and energies involved in bonding, realistic dynamics of the atoms can be calculated and displayed graphically and haptically to the user. To create realistic dynamics, the standard bond length and energy values were scaled and a simplified force feedback model was used. This provides the user with forces that feel natural and update quickly in both environments. The standard tables containing the bond lengths and bond energies were used to develop realistic force and distance

relationships between the different atom combinations (H-H, C-C, O-O, C-H, C-O, O-H) [7]. Thus, force and distance ratio relationships hold true to real atom interactions and can be explored by the user.

3 Design

3.1 Program Framework

Our program was written in C++ and made use of the standard OpenGL graphics libraries. The main program served to update the graphics and capture any keyboard input from the user. The position of the user is sensed using the PHANTOM and indicated visually by a small cursor within the virtual world. This cursor may act by picking up and dropping atoms; when not holding an atom, there is no force delivered to the user. Each atom within the program was instantiated as an object of the class atom, a new class defined for this project. The control thread, running at 1000 Hz, used the PHANTOM position and atom properties to compute interaction forces.

There are four possible states for an atom in our simulation. The default status is *unplaced*, an atom that is neither bonded nor being actively manipulated. In this mode, an atom did not contribute to the forces on any of the other atoms. Another possible state is *held*. In this case, the user is manipulating the atom; its location is the same as that of the user's cursor. This atom applies force to any other atom within a predetermined area. In addition, it experiences forces from other atoms in the simulation, allowing the user to feel the forces inherent in the simulation. A third state is *fixed*. Only one atom in this state exists in the simulation. This "ground" atom is fixed in space and still contributes to the forces on the surrounding atoms, but it is unaffected by the forces those surrounding atoms generate. The final atom state is the most important to the simulation – the *bonded* atom. These atoms apply forces to and feel forces from the surrounding atoms. In addition, they tend to move to the location of zero force, creating the behavior that one would expect from bonded atoms. It is important to note that these atoms are not kept at a fixed distance from other atoms. Instead, they are held in position by the forces that they are currently experiencing.

3.2 Simplified Model for Force Calculations

During each iteration of the control loop, the forces between every atom of the last three types (held, fixed, and bonded) are calculated. The positions of the bonded atoms are then updated if necessary. The interaction of atoms in the real world is quite complex. Numerous theories exist to explain exactly how such atoms interact and they attempt to reproduce all observed behaviors. In our project it was necessary to utilize a model that could be used at a high servo rate for stable and smooth haptic interaction. Further, this model needed to be used to quantify the interactions between all the active atoms in the world - and each atom interacts with every other atom. This requires a total of $n!$ applications of the model (where n is the total number of active

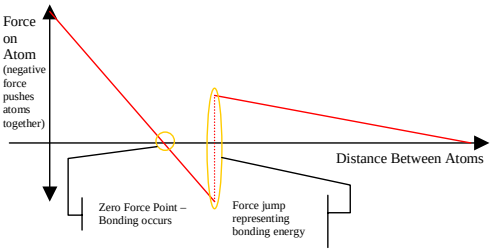

Fig. 3. Diagram of the force applied using the simple model

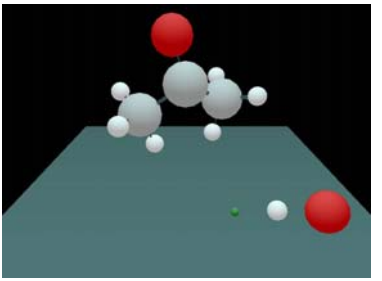

Fig. 4. A molecule (Acetone) built with the simulation

atoms in the simulation). In creating our simplified model, we kept in mind the educational context, so it was not necessary to reproduce all behaviors exactly. Most of the nuances of a very complex model would be lost during the transition to force output.

The final model incorporated in the simulation is shown in Figure 3. The model consists of two major regions. At some distance from the atom, the force experienced is positive, indicating repulsion of any nearby atom. At closer distances, the force becomes first attractive and then repulsive. In between the extremes there is a point at which the atom experiences no force. This is considered the optimum bonding distance for the atom. An atom dropped near this point will be considered bonded to the nearby atom and remain held in position by the forces experienced. This model is only active for atoms that could possibly bond. In cases where one atom has already been bonded to the maximum number of atoms (its valence shell has been filled), there is only one direction of force, always positive. This indicates repulsion, increasing linearly as the atoms are moved closer together. By using these two models, it is possible to obtain a simulation that reproduces most of the first order effects observed in the real world. While some small nuances may be left out, the simulation retains the ability to allow users to feel the major forces on the atoms.

4 Simulation Performance

The system was first shown to over 50 people at a public demonstration. The attendees had varying degrees of experience with haptics, robotics, and chemistry. In general, the reaction was very positive. Most people felt that the interface was very intuitive and enjoyed building molecules with the program (Figure 4). Several comments were made that allowed beneficial changes to be made in the program before the actual experimental trials, such as the inclusion of a positive sound allowing the user to easily tell if they had successfully bonded an atom.

In order to test the simulation, we created an experiment that would allow us to see how force feedback affects molecular creation in a virtual environment. We chose two different molecules for subjects to create using our program: methane (simple) and ethanol (complex). Each molecule was built several times under two different feedback conditions and the assembly time was recorded. In the first condition, the

user felt the force feedback that had been designed into the original program. In the second condition, force feedback was removed. Each subject built each molecule three times under each condition, resulting in a total of 12 molecules built per subject. In order to eliminate skewed results due to learning how to use the program, the users were allowed up to five minutes to interact with a single atom in the program. This allowed them to become familiar with the boundaries of the workspace and the procedure for picking up and dropping an atom. However, with only one atom in the workspace, the users were unable to experience any force feedback from atom-atom interactions; this was an important aspect of the experiment. The ten subjects who participated in the experiment were equally divided into two groups. The difference between the two sets was which feedback condition that the group experienced first. Group A was given force feedback at first, then no force feedback for the second set of trials. Group B experienced the reverse order of feedback.

5 Results

At first analysis, the average times for the two feedback conditions reveal no obvious differences between the sets of times, apparently indicating that force feedback has no effect (Figure 5). In order to verify this, a two-way ANOVA was performed to indicate any true correlations. The two factors were the feedback condition and the type of molecule (see Table 1 for the p-value results of all the ANOVAs performed). The results of this test appear to correspond with the initial conclusion drawn from simple observation of Figure 5, that there is no correlation between feedback type and the assembly time. There is a very strong correlation between type of molecules and the time required to construct it, as expected from the difference in complexity between the two models. Interestingly, there appears to be some interaction between the two variables. One possible explanation is that a more complex task benefits more from force feedback then a simple one.

A more interesting result is obtained when the two groups are examined independently. In Figure 6, Group A performed the task with force feedback first, while Group B received no feedback first. In Group A, there again appears to be little or no effect from force feedback. The results of the ANOVA test back up this observation,

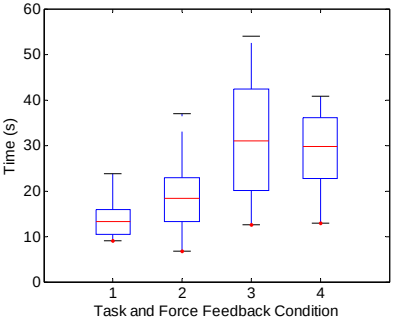

Fig. 5. Time required, averaged over groups A and B. On this and the following two plots: 1 - methane with feedback, 2 - methane with no feedback, 3 - ethanol with feedback, 4 - ethanol with no feedback

Table 1. Two-Way ANOVA Results

Factor	Groups A & B	Group A	Group B
Feedback type	0.645	0.3155	0.0078
Molecule type	0.0	0.0001	0.0
Interaction	0.0614	0.3562	0.0294

showing a high p-value. However, in Group B, force feedback has a noticeable impact. The ANOVA test shows that this impact is indeed statistically significant; the low p-value indicates that force feedback has a large bearing on creation time. There is also some interaction between the type of molecule and the type of feedback.

It is possible that the time to build each molecule may have been skewed by the learning curve inherent in this task. First time users of the program will obviously take longer to perform a task then those who have already experience the environment. However, in this experiment we have introduced several compensatory measures. The first is the training period mentioned earlier. The second is that last two of the three trials were used in the statistical analysis. These measures appear to remove much of the learning curve, as can be seen by the ANOVA results of group A.

From these results, it appears that force feedback can have a significant impact on the speed a molecular assembly task. When feedback was given first, the time required to build a molecule jumped to one level and appears to remain constant even when feedback is removed. Subjects retained their ability to assemble quickly even when force feedback was removed.

6 Future Work

Our atom builder is a tool that incorporates the use of 3D graphics and haptics to create a virtual environment that we cannot ordinarily interact with in the real world. The simulation program is an initial step in using nontraditional methods to teach novice students the underlying principles of molecular biology/chemistry. While the haptic simulation presented in this paper is effective, several enhancements can be

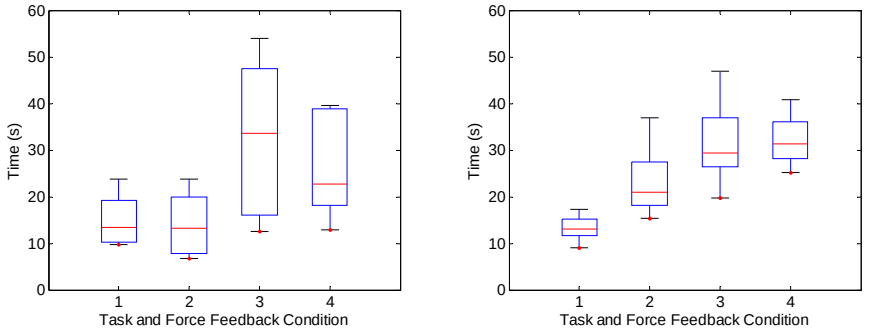

Fig. 6. Time required to build the molecules; left, group A only; right, group B only

made to make the program more versatile and robust. The most natural addition would be the incorporation of more complex molecules and their associated geometric features, such as double and triple bonds. Additionally, our simulation could also be extended to include chemical reactions. This would enable the user to experience a different type of atomic bonding and use the simulation to develop fundamental chemistry knowledge. Finally, the simulation environment itself could be expanded to create a more three-dimensional sense of immersion through the use of virtual reality and other simple, but non-invasive, devices.

In addition to the slight modifications, it would be most beneficial to verify the effectiveness of the simulation in comparison to the traditional teaching methods mentioned in the introduction. While the experiments conducted in this paper show the benefits of haptic feedback for exploring atomic properties, they don't compare it with the traditional methods of teaching mentioned in the introduction. Therefore, we are currently designing an experiment to determine the effectiveness of our simulation program. We would like to test the hypothesis that our simulator, as an interactive learning tool, will help the novice student learn and retain the fundamentals of chemistry in a more enjoyable fashion. We plan on testing our hypothesis on fifth grade students at a local elementary school. We will introduce some very basic concepts of chemistry and then let some of the students try the haptic simulation while other students try preexisting methods. Using subjective feedback from the classroom, we will be able to fine tune to model and explore whether or not the interactive simulation increases the students motivation to learn. By analysis of student performance, we may be able to grasp the educational benefits of applying haptics to learning and retention.

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