Scientific Visualization for Undergraduate Education

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Introduction

It has been said that one of the greatest challenges for students learning subjects in STEM is the need for the ability to think in three dimensions [1]. However, these skills are typically underdeveloped in undergraduates, even in the best of students [2]. Even though there is widespread need of students to understand and visualize spatial relationships [3], surprisingly little work has been done in the field of education to address this need.

Hardware to accomplish this goal has been in existence for several decades, though only since 1993 has it seen applications in education [4]. Educational advances have increased since that time, albeit slowly. Important advances include Christopher Dede's application of visualization hardware to general scientific concepts [5], and the teaching of electromagnetics in particular with the well-known MaxwellWorld [6]. Other applications include education of elementary school students in basic zoological concepts at Georgia Tech [7, 8], the NICE project for elementary education at the University of Illinois at Chicago [9]-[11], and engineering education research at East Carolina University [12].

This paper describes the efforts at Valparaiso University to augment students' education in several areas of science, mathematics, and engineering by using three-dimensional visualization hardware. Utilizing a newly available, low-cost system, the advances here promise wide-spread application due to the financial feasibility of this hardware to most universities. We discuss several custom-developed applications, in addition to their use in undergraduate courses.

Hardware System

In the past decade, visualization systems have cost from $300,000 to several million dollars. On the low end, companies such as FakeSpace (www.fakespace.com) have made available such devices as a one-user ImmersaDesk, offering a display of roughly three by four feet. High end systems such as the 6-walled CAVE at the University of Illinois at Urbana Champaign utilize 10'x10' walls on all sides of the user to create a truly immersive effect. Such systems can cost on the order of $10M.

Due to the high cost of such systems, most work done in visualization has not focused on education. The investment required to purchase visualization systems has been out of the reach of most teaching-oriented schools, and has not allowed them to be prevalent in classrooms. However, within the past few years, low-cost devices offering much of the functionality of classic systems for one or two orders of magnitude less in cost have become available. These devices are based on commercially available commodity computer hardware, only recently powerful enough to drive graphics-intensive applications. Such systems are typically PC-based utilizing a high-end graphics card and LCD projectors. These devices project a three-dimensional image onto a large screen, giving the user a sense of immersion and allowing a

person to see depth through binocular disparity. An overview of current hardware is given in [13].

The system used in this research is the Visbox virtual reality system, manufactured by Visbox, Inc. (www.visbox.com). It consists of an 8'x6' screen with dual projected images which are filtered so as to present a different image to each eye. In addition, the system includes a tracked user-interface device (a "wand") which allows the user to interact with the programs in six degrees-of-freedom. Finally, the user wears tracked glasses which allow the display to customize the image to the viewpoint of the user.

Chemical Visualization

A mechanical engineering course in materials science taught at our university involves studying unit cells of crystalline material. To support this course, we developed an application to show these structures at the atomic level. A representative screen shot from application is shown in Figure 1. The user is able to show unit crystal cells in cubic, body-centered cubic, face-centered cubic, and hexagonal form. A three-dimensional pointer allows an instructor to reference various aspects of the structure, or for a user to select atoms to show the associated Miller Index or slicing plane defined by the selected atoms. In addition, the sizes of the atoms can be increased or decreased from full size (atom shells touching adjacent ones) to zero radius. To show the concept of doping, interstitial atoms in octahedral and tetrahedral sites can be toggled on and off and can be assigned different colors.

An associated application allows a user to create his own crystalline structure by specifying the location, radius, and color of each atom. The specification is given in a text file, which is simple to generate. Using this generic interface, one instructor was able to create an illustration of crystalline silicon (the zinc blende structure) within five minutes and demonstrate this to his class. Alternate hexagonal rows were colored red and green to show the tiling of the underlying face-centered cubes. In this way, the silicon crystal structure was compared to the diamond form of carbon to illustrate the similarities. The graphite structure of carbon was also shown as a comparison.

Also available on our system are two comprehensive chemical modeling packages. The first, Visual Molecular Dynamics, has been ported to the Visbox system. This is a generic chemical visualization package, allowing the input of standard file formats such as .pdb (protein data bank). This allows us to download any of thousands of prepared molecule structures and display them to students in three dimensions. Several representations are available for each molecule, such as ball-and-stick, bonds, or points-only. A second package, called Ribbons, was developed by M. Carson at the University of Alabama, Birmingham. This has been ported to the Visbox, and is specifically designed for the visualization of protein molecules. An example application shot is shown in Figure 2.

All three of the chemical visualization programs were used to augment a course entitled "Elementary Physical Chemistry" in the fall of 2003. Students viewed organic molecules and proteins using the various software packages. In addition, they were able to download their own protein database files and bring them into the visualization laboratory. Molecules or structures they were having difficulty understanding were prepared and shown on the system.

Vector Fields

A challenging concept for many of our students in our third calculus course involves the visualization of three-dimensional vector fields and associated curl and divergence. Typically, students see formulas for a vector field such as

$$\left\langle \frac{x}{x^2 + y^2 + z^2}\hat{i}, \frac{y}{x^2 + y^2 + z^2}\hat{j}, \frac{z}{x^2 + y^2 + z^2}\hat{k} \right\rangle$$

and have no feel for the nature of the field, let alone the meaning of the curl or divergence of the field. The application developed shows three-dimensional Cartesian Coordinate Axes and draws arrows representing the field at each point. The size of the arrows and resolution of the vectors can be increased or decreased. A toggle is available to show the curl, which appears as an alternately colored vector originating at the same point as the field vector. One thing that becomes immediately clear to the student when showing the curl is the fact that it is always perpendicular to the vector field itself.

This application was demonstrated to two sections of Calculus III. Students attended smaller lab sections of 6-8 students and were shown ten different vector fields. Before each field was shown, students were asked to describe what they felt both the vector field and associated curl and divergence would look like. Some field specifications were easy to see from the equations that the divergence or curl was zero, but the students were not able to describe the vector field which resulted in this. By seeing both the manifestation of a specified vector field and its associated equation, students were able to gain greater insight into the relationship between the equations, operations, and manifestations of the fields they had been studying.

Electromagnetics

One daunting task for most students is to take an equation for a phenomenon and tell what it "means" or what it "does." This is especially true in the area of electromagnetics, where Maxwell's equations have befuddled generations of students. Take for instance the equation for the electrostatic field due to a point charge:

$$\vec{E}(\vec{r}) = \frac{q}{4\pi e_0} \frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|^3}$$

Though compactly expressed in this form, students often do not have a good feel for the physical manifestation of this field, especially when other point charges are added. Though the vector fields simply add due to the principle of superposition, students have difficulty grasping the interactions between various charges.

The application developed to illustrate this concept to students studying Coulomb's law consists of the following. An arbitrary number of point charges are placed in space. Each charge carries an associated magnitude which can be set. The application then plots the vector field resulting from these point charges. A three-dimensional cursor allows students to place a test charge at any point in space. By releasing the test charge, students can view the charge flowing in the field under the forces created by the static charges. Test charges are repelled by positive charges and attracted to negative ones. Test charges are always eventually attracted to a negative charge. A "bread crumb" trail is left behind to mark the path of the test charge.

We have found three main realizations that students immediately realize through interacting with this application. First, that the electric field lines created by the paths of the test charges never intersect. Second, that the standard dipole picture they see in textbooks can be generalized to three dimensions. And thirdly, that lines of equilibrium shown on a two-dimensional drawing can be generalized to a three-dimensional equilibrium surface. Students generally like trying to find and plot these equilibrium surfaces, as the action of the test charges is quite animated around these points. Students also get the feel that the electric field acts much like a gravitational field (one that they have an easier time visualizing). It is important to then impart to them the fact that both phenomena follow an inverse-square form.

Evaluation and Lessons Learned

We have found that there are two modes for using this technology in the classroom. The first mode is for content-delivery and demonstrations. In this mode, a group of students are passive observers and an instructor illustrates concepts. For this type of presentation, it is important to have a large enough space for the students to congregate, but also an intimate enough setting so that students can be close enough to the screen to have as much of their field of vision taken up by the screen. This also helps with engagement. The tracked wand is essential for presentation in this case, as it is the main device with which the instructor can direct student focus.

It is important to note that head tracking, or the customization of the display for a particular participant's viewpoint, is not a factor in this application, as several individuals are viewing the scene at once. It is even distracting for the group at large, and this feature should therefore be disabled. The issue of immersion, a key goal of most virtual reality systems, is also not a factor in this situation.

The other educational mode used with this system has been allowing an individual student to interact with the system. This is especially applicable in programs such as the electromagnetic field simulation. The learning in such cases is best done by discovery, where the student can interact with the field, change charges, and see the results. Though it is logistically difficult to arrange for many students to learn in this way due to the availability of only one system, the mode is still important. In such cases, the head tracking and associated immersion is very important. The needs of the system are much more akin to the classic pursuits of virtual reality systems.

Seeing that the needs of the display are different for the two situations, it is important to analyze two commonly available configurations for low-cost systems. A three-dimensional display only, such as the GeoWall system, has approximately one-half the cost of Visbox system due to the fact that it has no head tracking or tracked wand. The drawback of a GeoWall system in education is the unavailability of a tracked wand, which we have found to be indispensable for both group teaching and individual demonstrations. The benefit, of course, is the lower cost. Unfortunately, there presently exist no middle-ground systems that have no head tracking but do have a tracked wand. This is largely due to the fact that the cost difference between the two systems springs primarily from the electronic device to track the wand. The cost of head tracking is minimal compared to the cost for this feature.

Conclusions

The need for students to be able to visualize in three dimensions is essential. Current low-cost visualization systems offer great promise for education in that they are cost-feasible and hold promise for new pedagogical methods. The applications described herein have been successfully applied to undergraduate education and form a basis of future work. System capabilities of visualization systems are driven by the application, and it is found that for classroom instruction, it is necessary to have a tracked wand interface.

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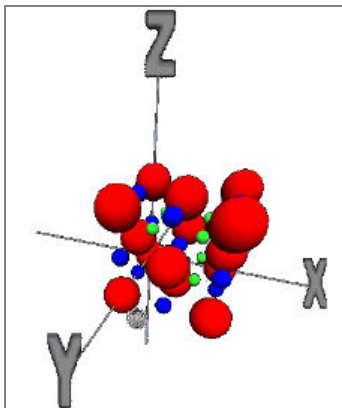
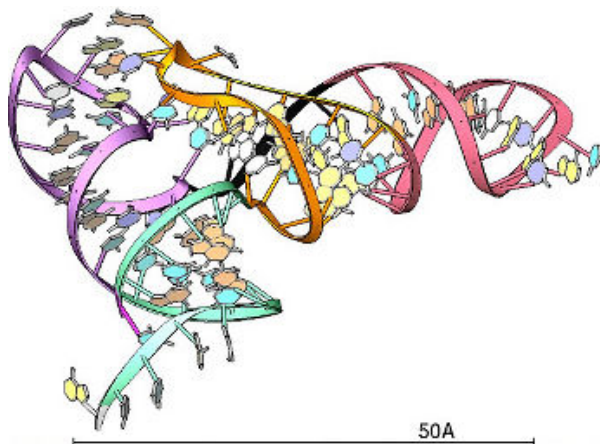**Figure 1 Application to show a face-centered cubic structure with interstitial atoms.**

Figure 2 Protein molecule shown by the Ribbons software