A Stereographic Table for Biomolecular Visualization

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Abstract

An inexpensive, stereographic table has been built to support molecular visualization with mainstream software that runs under Microsoft Windows. Indeed, any Windows-based software that supports side-by-side stereo pairs can be easily run on the stereographic table. This paper presents the table's design, construction, costs, and initial user experiences.

1. Introduction

Chemists have long relied on stereoscopy to convey a sense of space and structure. As early as 1926 von Laue and von Mises [1] published a set of cards with stereoscopic line drawings of crystal lattices. In 1965, Carol Johnson's ORTEP program revolutionized molecular display by guiding a pen plotter to create line drawings of molecular and crystal structure stereo pairs [2]. Today, PC-based molecular visualization software routinely renders interactive stereoscopic pairs. In particular, many Microsoft Windows applications are direct ports of their Unix workstation predecessors [3-8].

Unlike general-purpose data visualization environments such as OpenDX [9] and AVS [10], or visualization toolkits like VTK [11], molecular visualization software is domain specific, and in many cases, rendering is tightly integrated with data generation. Much research grade software is freely downloadable, thus transforming the software side of molecular visualization to a near zero cost process. Common to nearly all systems is that rendering functions are programmed in OpenGL, and interactive side-by-side stereo pairs are displayed in a single window.

OpenGL provides a rich library of rendering features that are used for display of traditional molecular representations such as ball-and-stick, space filling models, and protein ribbon representations, as well as orbital and electron densities with texture mapped isosurfaces and volumes. And since OpenGL is supported on a wide range of video cards from gaming cards like the ATI Radeon to CAD-Visualization cards such as 3Dlabs' Wildcat, molecular visualization programs may be used productively on any PC.

Stereo pairs present a particular problem for CRT viewers because stereoscopes can not be used at a typical viewing distance of 18 inches. The ideal solution is to use active stereo shutter glasses. However, there are two problems. First, not all molecular visualization packages support shutter glasses. Second, projective stereo viewing employing active stereo glasses is prohibitively expensive for groups. Alternatively, users can view stereo pairs without hardware assistance by resorting to free viewing.

There are two methods of free viewing: parallel and cross-eyed. A parallel viewing observer first isolates each image for its respective eye, then gently releases the eyes for image fusion. In crossed eye viewing, left and right eye images are images are juxtaposed by gently crossing the eyes. Unfortunately, about 2% of the population is stereoblind and is unable to fuse pairs by free viewing. And, although most molecular visualization packages can be set to render either parallel or cross-eye pairs, shared viewing among mixed skilled users is problematic. Yet, side-by-side stereo pairs are perfect for passive projective viewing. In particular, it is possible to build a projective stereo system without the need to modify software.

The core component of a projection-based passive stereo system is a dual display. Figure 1 shows a sche-

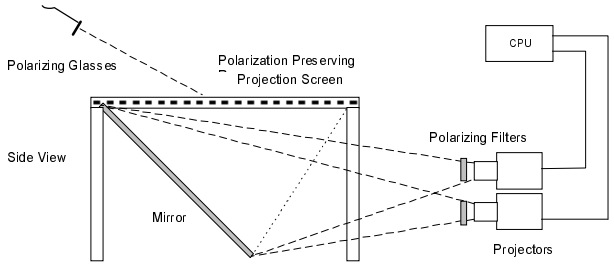

Figure 1. Diagram of 3D stereographic table.

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matic diagram of a stereo table where left-right stereo pair images from two projectors are superimposed on a rear projection screen. Left and right images are placed on separate displays by stretching the single window that contains them across the Windows' desktop from the minimum to maximum extents so that each stereo half-window occupies an entire display. The advantage of this system is that any user can open an application for shared stereo viewing with no further intervention. Building the stereo display system into a stereographic table enables shared interaction in a small space.

A stereographic table was designed and built to test the viability of a projective display system with respect to four design guidelines:

- It should be inexpensive to build.
- It should be small enough to fit into a small laboratory or large office.
- It should support multiple viewers.
- It should be easily disassembled, reassembled, moved and stored.

The following section contains a review of related work. Section 3 contains the table design and implementation. Section 4 provides a discussion and the last section suggests future research.

2. Related work

The three most notable stereographic tables are EVL's Immersadesk,[12] Kreuger and Froelich's Responsive Workbench,[13] and UNC's Nanomanipulator.[14] These systems, and the systems manufactured by companies like Fakespace and Barco, are expensive and require high-end computer systems to properly drive them.

PC-based stereographic projection systems have appeared, but use Linux as the operating system. For example, Jones, Parker, and Kim have built a Linux PC with dual-head display for passive stereo projection on a silver lenticular screen [15]. Open-DX is used to visualize 3D vector fields in plasma physics. AGAVE (Access Grid Augmented Virtual Environment) at EVL is a rear projection passive stereo system for large groups. It runs on Linux-PCs employing the CAVERNsoft library[16].

3. Table implementation

There are six components to the stereographic table: table framework and mirror, rear projection screen, projectors with polarization filters, video card, pointing device, and visualization software (Figure 2). They will be discussed in sequence.

The table frame was designed to be simple to construct. No woodworking facilities were available for construction. A 39"x 51" rectangular frame was built to support a screen with a 36" x 48" viewing area from 2"x 4"

Figure 2. Stereographic table as constructed.

lumber cut to the required lengths at a local lumber supplier. Frame parts were butt-joined with steel mending braces and screws: four straight braces for outside joints and four 90° braces for inside joints. Screw-in detachable legs with casters were added to complete the structure.

The screen was sandwiched between the wooden frame and a 1/4 inch sheet of clear acrylic held in place by four squeeze clamps. This produces a rigid structure because the screen's aluminum frame adds significant overall stiffness. The mirror is not attached to the table, but leans against the front two legs. Its length is such that when its top edge is set against the leg's highest point, the mirror makes a 45° angle with the screen. The mirror is standard silvered glass, 36" x 48" by 1/4 inch thick. It resides in an aluminum frame, backed with 1/8 inch acrylic for additional rigidity.

The rear projection screen is a "Disney" Black polarize-preserving screen with a "Snapper" mount from Stewart Filmscreen Corporation. The screen snaps onto a 39" x 51"x 1.5" sq., black aluminum frame to create a 36"x 48" display area.

Two NEC VT540 1000 lumen LCD projectors were selected for the system. They have native XGA resolution (1024 x 768), are reasonably priced (approximately $3200 each), and provide extensive control over the projected image including: positive and negative keystone correction; front, rear, ceiling, and table mounting; and independent adjustment of rgb color channels.

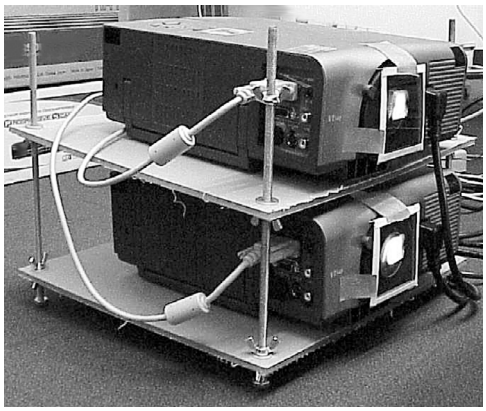

Figure 3. Detail of projector stacker.

The two projectors were stacked to superimpose left and right images. An adjustable support structure was constructed to align projection beams built using two 15" x 15"x 0.25" acrylic sheets and four 12" rods with 3/8" screw threads running their lengths. Holes were drilled at the corners of the acrylic sheets to accommodate the rods. Each sheet supports a projector and is easily adjusted using wing nuts (Figure 3).

Standard, three-inch square linear polarizing filters were installed in front of each projector lens, set orthogonally at $\pm$ 45°. Filters and plastic framed linearly polarized glasses were purchased from Reel-3D Enterprises. Linear polarizers transmit approximately 38% of the projector's illumination. Given an image created by two 1000 lumen projectors, the maximum expected image brightness is 1000 x 2 x 0.38 = 760 lumens. This is sufficient for viewing in a dimly illuminated room.

Microsoft Windows 98, 2000, and XP Professional support multiple displays either with multiple video cards, each attached to a separate display, or a single video card controlling multiple displays. A Matrox Millennium 450 was selected because it is an inexpensive mainstream graphics card that drives two displays, and supports OpenGL. A signal splitter was attached to each display connector to send signals to both a monitor and projector.

The pointing device is a GyroRemote by Gyration. The GyroRemote is an in-air mouse that detects hand motion and coverts it to cursor movement. The remote uses radio frequency to communicate with a base station attached to a PC's USB port.

Prices and total cost for the stereographic table are found in Table 1.

The table was connected to a Dell OptiPlex computer with a 900Mz Pentium III processor and 256MB of memory running Microsoft Windows 98. The system was tested with three freely available molecular visualization programs: VMD, Accelrys ViewerLite, and SwissPDBViewer. Figure 4 shows an image of a solvent accessible surface of the protein relaxin color coded by electrostatic potential running on the table rendered by Viewer Lite. Two LCD monitors are above the table displaying the left and right images that are superimposed on the table.

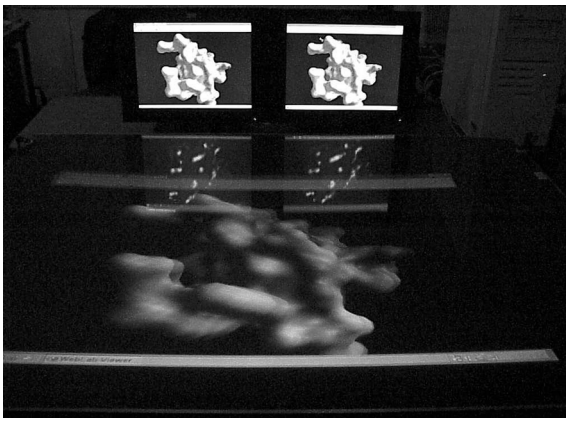

Figure 4. Sterographic table showing a stereo image of protein relaxin. LCD panels (at top) display left and right images.

An interactive session begins with loading the visualization software and extending the software window across Window's desktop until it fills both displays. A protein file is loaded and the software is set to render in stereo mode. ViewerLite creates stereo pair images in two halves of a single window. When the window is resized, the software automatically re-centers each image and adjusts its aspect ratio. No further user intervention is required. If the projectors are properly aligned, a pronounced stereoscopic effect results. VMD works in the similar fashion, and extends contol over the camera's angle of view. In contrast, SwissPDBViewer requires the user to reset stereo pair separation by adjusting the number of pixels between views.

Table 1. Stereo table component costs

Qty.	Item	Price
2	NEC VT540 LCD Projectors	$ 6,400
1	Rear Projection Screen	662
1	GyroRemote Mouse	180
1	Matrox 450 video card	137
1	Silver Mirror	117
2	VGA Signal Splitter Cables	110
4	Lumber, Legs with Wheels	81
	Acrylic Sheets	69
	Clamps, braces, picture frame, etc.	107
	Linear Polarizers (2), Glasses (4)	52
	Total	**$ 7,915**

4. Discussion

Discussion of the table will be broken down into two parts. First, a discussion of how a group of individuals

interacted with the table. Second, an evaluation of the table's component parts.

4.1. Observation of users

Stereo table use was informally monitored with a group of eighteen individuals, 20 to 65 years of age, and ranging in height from 5'4" to 6'5". Each session was about ten minutes long. None of the individuals had had data visualization experience, and few had any recent involvement with chemical imagery.

Users were allowed to view and rotate several proteins and DNA structures in three representations including stick, ribbon, and solvent accessible surface. Stick figures are wireframe representations where all bonded atoms are connected by an edge. Protein structures typically have highly irregular shapes, built-up from hundreds or thousands of atoms, each bonded to three or four nearest neighbors. As a result, a protein stick figure resembles a deformed bird's nest of densely packed lines rendered in red, white, blue, and gray. A ribbon model represents a protein's structure by fitting a spline surface through its amino acid backbone. Solvent accessible surfaces show the points of closest approach a water molecule makes to the biomolecule's surface. Surfaces appear as if an elastic membrane has been stretched over hard spheres placed at each atom position (Figure 4). Surface regions are colored red or blue if there is a significant positive or negative potential energy of interaction. Ribbons and surfaces were displayed using OpenGL's Gouraud shading and intensity depth cueing. Stick figures were intensity depth cued.

It was found that all viewers could sense the stereoscopic effect. Indeed, nearly all viewers exhibited a "grab" response, attempting to touch a stereo image, as it was perceived to protrude above the table. The stereo images that elicited the most active user response were the molecular surfaces. These were followed in turn by ribbon representations of proteins and DNA and lastly, stick representations. It is possible that a certain amount of stereoscopic accommodation took place as each user worked with the table. For example, some users had initial difficulty seeing the traditional ladder representation of DNA in stereo, but immediately perceived its helical shape when a surface representation was substituted. When the ladder model was displayed again, viewers could fuse the image pair.

Protein stick figures displayed near the end of each session were the most difficult to visually understand. These molecular visualization programs draw bonds with single pixel diameter lines, so projector misalignment makes stereo fusion more difficult. The two projectors used here were not perfectly aligned. Even so, by the end of each session, viewers could see stick figures stereoscopically and described what they saw.

Users were neither told what molecules would be displayed nor what a visual representation meant. Yet some people readily recognized structural features. For example, when a solvent accessible surface of DNA, colored by electrostatic potential was put on view, it was recognized to be DNA, typically with the question: Is that DNA? The strong stereoscopic effect produced by the desk communicated the distinct ridges and valleys of the major and minor grooves and overall helical structure, without the need to resort to displaying a traditional iconic DNA ladder model.

Finally, an experienced structural chemist employed the table to visualize organic, inorganic, and biochemical structures. During a two-month period, the chemist spent approximately fifteen minutes a week using the table, comparing visualizations with those displayed without stereo on a 21" CRT. It was found that the larger stereo display made three dimensional aspects of molecular structure easier to perceive.

4.2. Table assessment

The stereo table cost nearly $8000 to build, with over 80% of the expenditure associated with projector prices. About $2500 could be cut from the total cost by using lower resolution SVGA projectors (800x600). In projected stereo experiments that proceeded building the stereo table, SVGA projectors produced excellent image quality. Therefore, if absolute cost is important, SVGA projectors are a viable alternative.

The table's width of 39" combined with the passive stereo display allows two users to work comfortably side-by-side. A third viewer can fit, but as each viewer moves toward the table corners, image distortion increases and polarization decays. The table's footprint is 39" x 84" including projectors. Ideally, a shorter depth would make the table easier to install in a small space. Raising the screen angle to 30° or 45° from horizontal would make viewing easier as well. Both of these issues may be addressed by redesigning the mirror system.

Projector alignment was enhanced by the stacker (Figure 3). Wing nut adjustment on each post made it possible to raise and lower any projector corner. However, placing both projected images in perfect alignment requires patience. It appears that for solid models such as protein surfaces, near perfect alignment is sufficient.

The Matrox 450 is designed for business graphics, and as a result its 3D graphics performance is insufficient for supporting smooth movement of molecular surfaces defined as polygon meshes. The board could be replaced with a more expensive CAD graphics card that supports dual display such as the 3Dlabs Oxygen GVX210. However, the Dell OptiPlex came pre-installed with a Nvidia GeForce 2 AGP card with 32 MB of VRAM. The Nvidia card was reinstalled and paired with a less powerful

Nvidia TNT2 PCI card with 32MB of VRAM from PNY (costing about $80). Each card drove its own display. Despite the mismatch, the two cards produced smooth rotation of complex protein surfaces.

Stereo table users must become accustomed to navigating the Microsoft Windows desktop during a stereo session. Dialog boxes pop up in either left or right display. Since both displays are superimposed, the cursor may appear to be atop a menu selection, but actually it is in the adjacent display. One solution to this problem is to place two displays near the table as shown in Figure 4. Looking up from the table toward the monitors, the user can assess cursor and menu positions. Practice is another approach. Over time the user becomes familiar with cursor movement and menu placement in the superimposed system, thus diminishing disorientation.

The GyroRemote in-air mouse worked well. It is not necessary to point the mouse at the receiver. To move the cursor, the user can point the mouse at the tabletop. A trigger on its under-side activates the mouse. The two mouse buttons reside atop the GyroRemote and are depressed with the user's thumb. The GyroRemote is not a six degrees of freedom tracking device, but it allows the user to focus attention on the tabletop. In particular, molecular visualization programs use the mouse to translate, scale, and rotate a molecule by dragging the cursor across the window. The in-air mouse easily replicated this desktop motion by waving it over the table.

5. Conclusions and future work

The table proved to be successful at delivering stereoscopic displays of molecular visualizations to groups of two or three users. Future work on the table will focus on applying it to the display of chemical dynamics simulations, running more general purpose visualization programs, and extending applications beyond chemistry. In addition, work is underway to redesign the table so it will be more compact.

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