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Comparison of Input Devices and Displays for Protein Visualization

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Introduction

For the visualization of proteins, interaction with the displayed model is indispensible in order to understand the three-dimensional protein structure. Accordingly, an efficient design of the user interface including display and input devices is crucial. A large number of input devices, some in 2D, some in 3D, and a large variety of display devices exist, which are commonly used for exploring large-scale 3D data structures. Unfortunately, not all combinations of input and display devices work together in a suitable and useful manner, either because they are not capable of 3D input or because, for instance, they need a hard table surface to work properly, making their utility for 3D navigation impractical. For example, in a large-screen, stereoscopic environment, where user immersion and freedom of motion in the display space are required, such a device would bind the user too much to a fixed location.

The purpose of this study is to provide an overview of existing technology and to identify combinations of input and display devices that have proven to work well together. The survey identifies capabilities and limitations of each technology. Even though they might have, for instance, sufficient degrees of freedom, we explain why some input devices are not suitable for accomplishing a certain task, or how they can be replaced by more suitable devices which allow more user-friendly and efficient solving approach.

In addition to the survey, a case study on protein visualization has been conducted. The application has been chosen because it incorporates complex navigational tasks, requires multiple degree-of-freedom user input, and gains from 3D stereoscopic visualization on a large, high-resolution display system. These requirements are typical for many scientific visualization applications as well as for games, the latter being the driving force for the development of cost-efficient VR solutions.

Multiple Degree-of-Freedom Input Devices

In many Virtual Reality (VR) applications, the software is required to facilitate multiple degree-of-freedom (DoF) tracking of user interaction. Sensors or controls of a tracking system usually provide information on the position and orientation of the input device in 3D space, where the position is given by the *x*, *y*, and *z* coordinates and where angles for pitch (rotation about the *x* axis), yaw (about the *y* axis), and roll (about the *z* axis) specify the orientation. Since not all applications incorporate all six degrees of freedom, input devices with less degrees of freedom might be more appropriate for some specific tasks.

Input devices for 3D interaction were first classified in [11]. An attempt to formalize the design, evaluation, and application of interaction techniques for immersive environments was made by [3], while a taxonomy for the design of 3D interfaces was compiled in [10].

Devices For Use With 6-DoF Tracking Systems

The simplest 6-DoF input device is probably the **stylus**. An integrated electromagnetic tracking system provides the desired information about position and orientation of the tip of the stylus, eliminating in most cases the need for a cursor, i.e. the virtual object can usually be 'touched', picked and dragged directly with the device. Due to its natural analogy, even VR-inexperienced users intuitively hold and use a stylus like a pen or laser pointer, and are able to pick a virtual object by pressing the single button on the stylus with the index finger. The stylus can also be mounted to a table-mounted, trackable force feedback device (e.g. the PHANTOM Omni by SensAble Technologies, Inc.).

Data gloves provide the user with an intuitive way to perform for more sophisticated picking operations, and, with certain limitations, quasi gesture recognition. Some data gloves feature resistance strain gauges for each finger. More basic types simply have metal contacts mounted to every finger tip, allowing for simple pinch gestures (**PINCH gloves**), used for interaction metaphors like "grab and move" and "grab and rotate". Although a large number of pinch combinations is theoretically possible, only a limited number is ergonomically feasible. Particularly, our experience has shown that the utilization of too many different pinch combinations or unnatural gestures in an applications often confuses the user.

The tracker is usually mounted on the backside of the cloth gloves, which results in a variable offset between the fingertips which grab the virtual object and the tracker location. This may cause actual objects to be occluded by the hand, making the use of a virtual cursor necessary if precise navigation is required. If a grabbed object is moved or rotated, the center of the rotation is usually the wrist of the grabbing hand. However, most applications use the tracker location instead of the wrist, causing a slight discrepancy between the pivotal wrist point and the actual tracker position as the rotation center. Techniques for bi-manual control of two independent cursors [21] might be necessary for collaborative or bi-manual interaction.

Pinch gloves are very suitable both in a tabletop and in a desktop environment, i.e. for use with virtual workbenches or smaller single screen displays ([15], [7], and [17]), which enable interaction with objects "in arms reach", but also for large-screen projection systems, provided that the wires that are usually attached to the trackers do not limit users in their freedom of movement. Some wireless solutions are currently under development.

Devices Without Additional Tracking Systems

Mice and **trackballs** are commonly used for one handed drag'n'drop and click'n'rotate interaction in 2D desktop environments, where the second hand can be used for activating additional functions (such as zooming in *z*, for example) through modifier keys on the keyboard.

Joysticks are also common input devices for navigation in 2D desktop environments. While the primary hand moves the stick in 2D and presses buttons on top of the stick, the secondary hand holds the device and manipulates additional buttons and throttles on the base. Two out of three translation or rotation directions (x, y, and z) can be selected and mapped to the joystick movement. Some joystick models also allow turning the stick, thereby adding an additional rotational axis. Additional degrees of freedom can be activated by pressing a button on the joystick or on the keyboard.

Steering wheels are usually only employed by applications which feature a driving metaphor, where the camera moves and no object has to be grabbed or manipulated. Navigating the virtual world like this is intuitive for exploration tasks of large virtual environments and worlds, but it is not suitable for VR-based space or desktop metaphors where the main focus is on object exploration and manipulation. Due to their size, weight, and design, steering wheels have to be mounted on a table.

Video game controllers can provide more flexibility than the above mentioned devices. A trigger and a jog shuttle on a Nintendo64 controller, for example, allow users to hold and handle this wand similar to a remote control by pointing in the direction of the screen. Although trigger and jog shuttle each provide only 1D axes, an additional tracking system can easily be mounted to the end of the wand, so that the VR object or the world origin can be translated according to the trigger orientation in the direction of the wand position or rotated according to the jog shuttle.

In recent years, **gamepads** have become the gaming device of choice. They come either wired or with a convenient cordless option, and feature up to two analog and one digital joystick plus sliders, thereby providing several axes for numerous degrees of freedom (DoFs). Four or more buttons are usually located on top of the device that can be reached by the thumb during interaction, while four buttons are located on the front of the device within reach of the index and middle fingers. A gamepad is similar to the joystick in terms of functionality and programmability. In both cases, two out of three degrees of freedom must be chosen to be mapped onto input devices that are 2D in nature (joystick, 2D digital pad). The navigation can easily be adapted to the habits and preferences of the user, since it is very easy to map a variety of navigation modes and keyboard functions to the interaction device.

Figure 1: (a) The PHANTOM Omni device by SensAble Technologies, Inc., (b) Microsoft SideWinder Force Feedback Pro Joystick, (c) Microsoft SideWinder Force Feedback Wheel, (d) modified Nintendo64 controller, (e) the Logitech© WingMan® Cordless Rumblepad.

Hand-Eye Coordination

For object exploration and manipulation tasks, desk-mounted devices employ an indirect mode of navigation, i.e. the user looks at the screen, not at the device, and navigates the cursor on screen by moving the device on the desk. On 2D desktop environments, most people adopt their hand-eye coordination quickly to this paradigm. In a 3D virtual environment (VE), however, this separation of hand movement and visual feedback seems to be much more difficult to adapt to. Preliminary studies have shown that most people find it more intuitive if they can interact directly with the object rather than using an indirect method. Video game controllers such as wands and gamepads are not desk-mounted and therefore can follow the movement of the user, thereby enabling direct object manipulation in immersive 3D environments similar to a stylus or data gloves.

Displays

A virtual environment (VE) is characterized by the display mode and the visualized information. Monoscopic and stereoscopic rendering provide the viewer with virtual depth perception and immersion into a virtual world. The degree of immersion depends on the projection type and the nature of the information which is supposed to be visualized. In general, a large display size allows several users to collaboratively investigate virtual models, provided that viewing of the model does not depend on tracking of an individual user in a virtual environment.

Multi-screen Projection-based Systems

The CAVE was the first available multi-screen setup for large VEs [6]. It is a multiple-screen projection-based virtual reality system with four to six screens that are arranged in a cube for total immersion. The most common setup consists of three walls and a floor. The major advantage of the CAVE is the fact that it enables collaborative exploration of several large-scale objects through manipulation and navigation within an immersive virtual world. Viewers navigate the virtual scene by naturally moving around inside the cube, while their field of vision is completely covered by the projected images.

Single-screen Projection-based Systems

Single-screen projection-based (SSPB) systems such as the Responsive Workbench (RWB) [**15**], Fakespace System's ImmersaDesk®, PowerWalls and Infinity Walls [**8**] consist of one screen, usually several feet in diameter, which is mounted at a variable angle. These Virtual Model Displays (VMDs) lack complete immersion, but guarantee excellent object presence. While the ImmersaDesk® utilizes a near-vertical pitch of the display surface, the RWB uses a tabletop metaphor, in which virtual objects appear to lie on the table's surface. This ensures easy accessibility for interaction with the data and allows intuitive interfaces to be shared by several users. The field of vision is limited by the screen dimensions.

Head Mounted Displays

Head Mounted Displays (HMDs) are mostly deployed in augmented reality applications. Some models are mounted on full helmets, which are too heavy for long time use, while others offer displays which are arranged in a position similar to eyeglasses. Not all HMDs support stereo viewing. HMDs are not optimal for all virtual environments due to their limited field of view, low resolution, and limitation to a single user. Since exact synchronization is necessary, collaborative work environments also usually do not employ HMDs.

Figure 2: (a) User in a CAVE-like immersive, virtual environment (COVE system at the Engineering Research Center at Mississippi State University) and using a (b) Virtual Workbench and (c) a Head Mounted Display (HMD)

Tiled Projection-based Systems

The resolution of most single projector systems is still rather limited. Therefore, multi-projector tiled displays with 9 (for 3x3 tiles) or more projectors can provide a substantially higher resolution than conventional screens [**20**]. Since several images are tiled over a single arbitrarily large display surface, overlapping areas have to be aligned [**4**] [**5**], and variation in color temperature and brightness eliminated through luminance matching [**16**].

Tiled LC Display Systems

Tiled LC panel display systems [13] consisting of 3x3 LCDs are a space-saving alternative, but are not stereo-capable and can not compare to an immersive environment, especially since their small size and technical nature prevent their use in a surround screen setup.

Figure 3: (a) and (b) Tiled 3x3 Projector Display with 9 projectors, (c) Tiled 3x3 LC Display

Preliminary Observations

The combination of input devices that require a desk with large, immersive, open spaces in a 3D display environment is not practical. Also, the combination of input devices that are 2D in nature with a stereoscopic display does not make use of the capabilities of the VR environment to the fullest extent possible.

Input devices that can be operated in an open space with one or both hands seem to be most suitable for 3D environments. Mixed systems, such as the Responsive Workbench, combine the table-top paradigm with stereoscopic rendering. However, a 2D mouse or a joystick, even though they are desktop-based input devices, are not suitable due to their lack of support for multiple degrees of freedom, and also due to their property of constraining the user to the surface of the table or to a particular location on the table.

In general, if the user task includes selecting and picking of objects, direct methods, such as grabbing using pinch gloves or dragging using a stylus, are preferable over indirect methods with disconnected hand-eye movement. Depending on the shape of the input device, a cursor or pointer associated with the input device and representing a single point used for object selection has been found to be helpful in performing precise navigation tasks.

Protein Visualization Application

The purpose of this case study is to explore various 2D and 3D interaction paradigms and their utility in analyzing the 3D structure of proteins, a task that requires 3D navigation, for example, translation in x, y, and z, and rotation about the x, y, and z axes. In addition, object selection by picking (using a push button or a similar gesture) is necessary to handle multiple objects. These tasks, as they occur in this particular application, have been chosen because they are typical for most applications in Virtual Reality.

Related Work

While rudimentary molecule structures have been previously explored in VEs ([17] and [1]), a large number of data sets of the 3D structure of macromolecules have only become available in recent years. They are archived in the Protein Data Bank [2]. Kinemage [18], RasMol [19], VMD [12], PyMOL [9], and MolScript [14] are software packages for molecule visualization. Most of these applications focus on the visualization of a single molecular structure with traditional mouse and keyboard interaction. We added new modules to MolScript, which is commonly used to generate high-quality visualizations for print publications, and enhanced the program with VR interaction support and options for comparative exploration of several macromolecule datasets in a variety of virtual environments (VEs) in real time.

Structure Determines Function

Protein visualization has been chosen because it is a typical example of an application where multiple renderings of an object from various angles and viewpoints may lead to new insights and a better understanding of how shape determines function.

Proteins are assembled through a sequence of 20 amino acids with different physical properties, including mass, surface, volume, solubility, and density. The order of these building blocks determines the 3D structure of the macromolecule. Interatomic interactions, chemical characteristics (polarity, size, acid or basic, hydrophob or hydrophil), and structural rules for spacing between atoms and bong lengths and angles also play an important role. Since the sequence determines the structure, it also determines the location of binding sites which are necessary to perform specific tasks. If the sequence and thereby the structure is changed, binding sites might become disfunctional or inaccessible, resulting in lost or altered functionality.

This relation between structure and function can best be explored by generating high quality 3D visualizations and by providing an intuitive navigation interface which allows for in depth inspection of specific details.

For a close analysis of a 3D protein structure, it is necessary to position and rotate the structure freely in space, with the possibility to explore the object from every angle and at various zoom levels. Since macromolecules with similar structures often have similar functions, a comparative exploration of several related structures is required, enabling a closer examination of similarities and differences through side-by-side comparison or superimposition, which might yield important information for understanding the relation of structure and function.

Molecule Representations

Detailed wireframe-like stick, ball-and-stick, or space-filling (CPK) representations provide details of the atomic structure, including information on volume, size, shape, and surface structure. Abstract schematic models can be given through so-called cartoon representations, which allow for easy identification of specific motifs consisting of β sheets (arrows), α helices (cylinders, helices), and loops (ribbons). Since the different models emphasize diverse aspects of the structure, a visualization of different representations is indispensable for a comprehensive analysis of the characteristical features of the structure and the surface of the molecule.

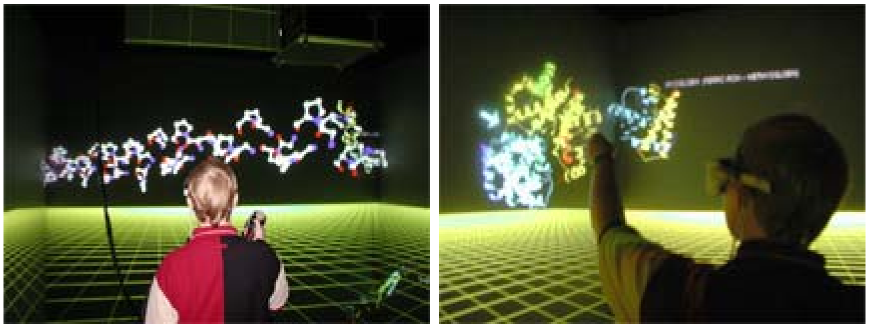

Figure 4: Exploring ball-and-stick and cartoon representations of proteins.

Protein Exploration

The protein visualization application focuses on the exploration of several large molecular structures in real time in an immersive virtual environment. It allows the user to compare several complex structures side-by-side or by superimposing them, and to position each structure freely in the virtual workspace so that details that may otherwise be occluded can be revealed. This is motivated by the fact that particular perspectives or orientations of a model may not be suitable for recognition of specific features.

The tasks required for a functional analysis of complex molecules are much easier achieved in VR than in commonly used, single-perspective, static or dynamic 2D projections. Since virtual objects may occlude each other so that individual objects are impossible to select by picking a specific point on the surface of the object, the interaction metaphors have to be adapted to allow for intuitive navigation. This implies that various methods for picking and moving of an object must be provided. For example, the center of rotation can be changed from the picked point to the center point of the object (or even to an arbitrary point in space), although the closer the center of rotation is to the object, the more natural and less confusing the navigation occurs to the user.

Input Devices

For our case study we surveyed various types of input devices to examine their suitability for exploring the characteristics of 3D protein structures.

Since our application did not employ a driving metaphor, but needed 3D interaction, the steering wheel was unsuitable for our purpose. The PHANTOM Omni, with its very limited interaction radius, also appeared to be inappropriate, especially since our implementation focused on protein visualization and exploration and did not include any simulation of physical forces, thereby eliminating the need for force feedback support. During the development of the application, we used the mouse for debugging purposes on our workstation. For short tests this was sufficient, but not for close and thorough inspection of details of the 3D model. The mouse was also limited to the desktop and therefore could not be used when standing in front of larger displays away from the desk. The same problem applied to the joystick. Especially larger models supporting force feedback were so heavy that they needed to be placed on a table surface.

The stylus was appropriate for grabbing or "touching" molecules in immersive setups where the 3D model seemed to float in front of the user. The stylus could be moved freely in space. If the button was pressed at a particular location, the closest molecule was grabbed and followed the movement of the stylus. The single button setup of the stylus limited the number of functions which were directly accessible to the user and made the use of an additional menu necessary.

The Nintendo64 wand provided more flexibility than the stylus. But even though this specific device supported up to 14 buttons (6 large buttons on the handle, 4 small buttons on the handle below the jog shuttle and 4 on the jog shuttle), not all of these buttons were ergonomically located. The users in our focus group too often had to look at the device to find the buttons and had difficulties to remember which function was mapped to which button since the buttons all looked similar and were not marked by a letter or symbol as on most gamepads. Since the location and similarity of the buttons was too confusing to some users, only a subset of the buttons on the device could be used. To ensure the intuitive handling of the application, we mapped the same functions to different buttons simultaneously. This was done in a separate experiment. The users therefore could operate the buttons on the handle with the dominant hand, but also select the same functions via the buttons on the jogshuttle with the other hand.

Gamepads in general exhibit a more balanced design. The users' hands always stay in the same position, where the thumbs operate the analog or digital joysticks and buttons on top of the device, and the index and middle finger are rested on the corresponding buttons on the front of the pad. All buttons are numbered or labeled with a symbol. This makes the ergonomically located buttons easier to press and the attached functionality easier to remember.
We used a cordless gamepad in our setup which allowed easier and unrestrained movement especially in front of large displays. In a 3D immersive environment, the users in our focus group tended to walk around the 3D protein models, step into the structures, and look through barrel motifs and helices. The cordless gamepad made it much easier for the group in the small space to walk around and to hand the device over to another user, because the users could not get tangled up in a cable loop.

The ergonomical design of the gamepad also allowed us to map a large number of functions and degrees of freedom to the numerous buttons and axes according to individual preferences, which made the gamepad the most flexible and easy to use device in our tests.

Finally, we also used a pair of pinch gloves to explore the protein structures. With the pinch gloves, touching, grabbing and moving a 3D structure directly felt the most natural to the users, because the virtual objects could be handled like real objects. This worked very well in immersive environments where the virtual 3D model seemed to float in space, but in non-immersive environments, where the object could not be touched or grabbed directly, the gloves did not show any advantage over other multiple degree-of-freedom devices. Since only grabbing an object by pinching the thumb and the index or middle finger is an intuitive gesture to most users, other functions associated with more uncommon pinch combinations often proved to be too awkward and therefore often too difficult to remember for some users. This limited the number of functions that could be used directly (without a menu).

Devices	**Wireless**	**Mounted / Needs Desk**	**Hands**	**Rumble / Force Feedback**
Stylus	No	No	1	-
Pinch Gloves	No	No	1 or 2	-

PHANTOM Omni	No	Yes	1	Force Feedback
Mouse	Optional	Yes	1	-
Joystick	No	Yes	2	Force Feedback
Steering Wheel	No	Yes	2, feet	Force Feedback
Nintendo64 Wand	No	No	1 or 2	-
Gamepad	Optional	No	2	Rumble

Table 1: Only computer mice and gamepads are available as wireless models for unencumbered interaction. Many devices need to be used on a desk, some with only one, some with both hands. Some devices are capable of rumble or force feedback.

Displays

In general, the choice of the display type depends on the specific requirements of the navigational tasks. Fully immersive VEs like workbenches or CAVEs are convenient for collaborative exploration tasks conducted by small user groups, who want to be able to walk around 3D structures and to inspect details of an object in close-up views. Only by total immersion in a stereoscopic environment can the users experience the full extent of the complex 3D structure of a protein.

Newer, tiled displays provide a much higher resolution for a clearer and more exact rendering of fine details. Not all of these displays are stereo-ready yet and therefore not capable of providing complete immersion. High-resolution displays are, of course, desirable, but not always affordable.

3D is a good solution to overcome screen clutter, even though the number of pixels on the screen is similar to 2D displays. By adding a third dimension, objects of lower priority can be pushed towards the background, eliminating the ambiguity of the zoom operation on a 2D display (size vs. distance).

Figure 5: The 3D structure of the enzyme Glutamine Synthetase (2GLS) as shown on a 2D screen shot, on a tiled projection-based system and on a tiled LC Display.

Some large display screens or display walls allow a command center-like setup, where a user sits at a desk a few feet away from the screen and uses a mouse or joystick to interact with the application. This is

impractical though if a lot of people are standing in front of the display, blocking the view from the command center to the screen.
Therefore, input devices that do not require a table surface are more suitable for collaborative protein explorations on large screens.

Our study showed that virtual workbenches, where molecules could be placed and inspected in a virtual workspace environment and where users could reach across the horizontal, table-like 3D display, were the optimal display setup to utilize the capabilities of the pinch gloves.
Even though the stylus also worked well with these displays, more functions could be mapped to pinch combinations than to the single button.

Users intuitively held the Nintendo64 wand like a remote control towards vertical displays. This worked well on large and tiled displays and in the CAVE. However, as mentioned before, the handling of this wand was not as intuitive as the handling of a gamepad, and since the wireless gamepad allowed the user group to move and hand the device around freely, the gamepad outperformed all other devices, especially since it turned out to be suitable for all display environments with vertically and horizontally mounted screens.

We did not test the interaction devices with the head-mounted display (HMD). Due to its low resolution and limited field of view, this display device proved not suitable for our protein visualization application.

Displays	**STEREO ready**	**Works with desk-mounted devices**
CRT	possible	yes
Workbenches (Horizontal or at angle)	yes	no
Single Screen Multi-Projector (Vertical)	possible	if control center-like setup
CAVE	yes	no
Tiled LCDisplay	no	if control center-like setup

Table 2: Not all display devices support STEREO or can be combined with a desk-mounted input device.

Conclusions and Future Work

We have presented an overview of applicable input devices and display systems for the exploration of protein structures in virtual environments in real time. The purpose of the study was to provide a survey of existing input and display devices and to draw conclusions with respect to their utility in various combinations. To explore 3D protein structures, the virtual environment should provide a large field of view, preferably at a high resolution, to show as many details of the macromolecular models as possible. Total immersion allows the users to examine the structures from different angles by walking around the models and grabbing and moving them around. Using simple and intuitive pinch gestures or ergonomically designed cordless gaming devices ensures intuitive and unencumbered interaction with the virtual proteins.

The lesson learned from the case study was that it is necessary to match a high-quality display device with suitable input device technology. A high-resolution, stereoscopic display cannot overcome the limitations of a poor input device to facilitate precise navigation tasks. Both input and display devices go together in enabling the user to complete a navigation task in a virtual environment in an intuitive way and with high precision.

In the future, ubiquitous computing and large-screen display environments will become more commonplace. New, emerging technologies such as high resolution projector displays, flat-panel displays, and OLED displays, will make it possible to access information everywhere and anytime. Interactive navigation using 2D and 3D input devices will become a critical component of this development.

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