Improving Collaborative Visualization of Structural Biology

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Abstract. Structural biology is the study of how molecular shape, chemistry and physics connect to biological function. This work is inherently multidisciplinary and co-located group discussions are a key part of the work as participants need to refer to and study visualizations of the molecule's shape and properties. In this paper, we present the design and initial assessment of CollabMOL, a collaborative molecular visualization tool specifically designed to support small to medium size groups working with a large stereo display. We present a task analysis for co-located collaborative work in structural biology in which we find shortcomings in existing practice as well as key requirements of an appropriate solution. In this paper we present our design of this solution and an observation based user study to validate its effectiveness. Our design incorporates large stereo display support, commodity input devices and displays, and an extension to an existing molecular visualization tool.

1 Introduction

Structural biology is the study of how molecular shape and physics connect to biological function. The work is inherently multi-disciplinary, as it includes both those who understand molecular geometry, and others who are interested in how proteins are used within biological systems. Co-located discussions are a key part of the work as participants need to refer to and study visualizations of the molecules' shape and properties. Our goal is to develop systems to support this collaborative visualization that are inexpensive and effective.

Collaborative molecular visualization is enabled by the availability of large, stereo displays. Such displays are becoming increasingly practical as consumer devices emerge. While current molecular visualization tools support a variety of displays, they are designed to support single user tasks, and are not necessarily well-suited for collaborative work.

Our premise is that group collaboration is best supported by software specifically designed to address the type of work being done. In this paper, we describe our experience developing a collaborative molecular visualization tool. We performed a task analysis to understand domain scientists' needs by identifying shortcomings in existing practice and key requirements. We used this task analysis to design a system that addresses these shortcomings and key requirements with low cost consumer displays and input devices. This design is implemented in a prototype which we use to a perform a user study in order to evaluate its effectiveness.

Contributions: Our primary contribution is to provide an analysis of the task of co-located collaborative molecular visualization, and the design for a system based on this analysis using commodity hardware. The specific elements of the solution may not be very novel. However, by basing the design on an understanding of the task we were able to tailor the solution, and better manage the tradeoffs in system functionality, cost, and usability. Together, the elements create a system that demonstrates that a task-informed design can produce an effective collaborative system. Our work also contributes a case study of how the design process can be applied to co-located collaborative visualization, and how tools designed this way can better serve user need than systems not specifically designed to support it.

2 Related Work

Several areas of related work influenced our design process including molecular visualization, co-located collaboration and 3D interaction methods.

2.1 Molecular Visualization

Structural biologists and their collaborators often use molecular visualization to gain a better understanding of the shape and other properties of the molecules that they work with. They utilize a variety of abstract representations of these molecules and visualization options in order to to best understand the molecule they are examining. Molecular visualization has a rich toolbox of visualization and analysis techniques. Donogue et al. gives an excellent overview of these techniques[1]. Some examples include ribbon representations[2], solvent excluded surfaces[3], ambient occlusion shading[4], and abstracted molecular surfaces[5].

There are several popular molecular visualization packages including VMD[6], PyMOL[1], and Chimera[7]. Because these tools provide a wide variety of visualization options and styles as well as analysis tools, scientists that work with them often invest a great deal of time and effort into gaining proficiency in their tool of choice. This allows them to quickly manipulate the visualization and perform the analysis necessary to make structure-function connections. Figure 1 demonstrates an example of the kind of visualization that they might create. This impressive depth of both visualization and analysis present in molecular visualization tools influences our design of an appropriate collaborative system.

2.2 Co-located Collaboration

Co-located collaboration refers to collaborative work that takes place in the same physical location. Previous work has explored a variety of display and interaction

[1] http://www.pymol.org

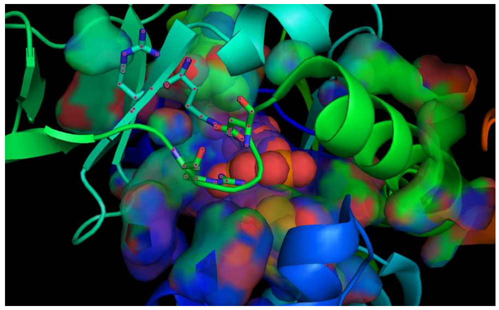

Fig. 1. This protein(PDB:1AKE) is rendered using a ribbons representation to show the secondary structure, a transparent molecular surface to show the shape of the binding cavity, a spheres representation to show the location of the ligand, and a sticks representation to show the location of residues near the ligand.

paradigms for collocated collaboration including immersive environments, table top displays, large tiled displays and multiple co-located displays. Other tools for collocated collaboration in the domain of molecular visualization include multiple immersive applications[8, 9], and a multi display collaborative adaptation of JMOL[10]. Our work deals specifically with the design of a single display co-located collaborative system for a specific application. Our experience and that of our colleagues has shown us that col-located discussions are common within the domain of structural biology. These and other existing collaborative applications help to inform our design process.

2.3 Bimanual Interaction in 3D Interfaces

Bimanual interaction has been shown to be an effective metaphor for interacting with 3D objects [11, 12]. The non-dominant hand is used for view manipulation which requires less precision while the dominant hand remains free for pointing and selection tasks which requires more precision. View manipulation is used not only to orient the view towards relevant objects but also to gain a better depth perception via motion parallax. Decoupling these tasks avoids constant switching between actions and facilitates improved perception of the object being explored and increases task performance [12].

3 Task Analysis

In order for our collaborators to do their work it is necessary for them to engage in group discussions of protein structure. They have found that these discussions are more effective when facilitated by a large, vertical, stereo display, as shown in Figure 2. These discussions typically revolve around specific properties of small pieces or areas on a protein molecule and are usually relevant to some other domain of study such as how the protein interacts with other molecules in a larger system. In order for these discussions to be effective they need to leverage the multitude of visualization and analysis options present in desktop molecular visualization software as well as their expertise in using the software.

In this task analysis we identified shortcomings of existing practice, key tasks, and functional requirements. In this section we discuss the key tasks we observed, the shortcomings of existing practice we observed and the functional requirements of the system.

3.1 Methods

We observed several collaborative discussions over a period of approximately six months. During these observations we noted how the existing system is used in a collaborative setting and how users spend most of their time. We noted road blocks to discussion and sources of confusion. We primarily used fly on the wall observation but if users encountered difficulties we asked them questions after they finished the session. In order to uncover other functional requirements of the system we discussed our plans with our collaborators.

3.2 Key Tasks

Our observations revealed that while many different visualization tasks are used, collaborative work in this area is strongly dominated by two key tasks: viewpoint control and pointing. Because each participant may prefer to tell their stories, moving between viewpoints is common, and considerable time is spent recreating previous views. In discussions, participants often use pointing gestures to refer to places on molecules. These gestures are done either with their hands or with the mouse pointer. Beyond the key tasks of viewpoint control and pointing we observed selection of sub parts of the molecule, switching between a set of selections and changing the visualization style of selections as important tasks that occurred frequently.

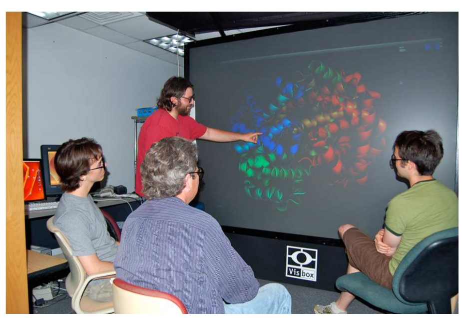

Fig. 2. A collaborative discussion we observed in our task analysis. The participants had a hard time understanding exactly what is being pointed at due to the parallax issue associated with stereo viewing.

3.3 Shortcomings of Existing Practice

Through our observations we observed several shortcomings of existing practice or roadblocks to effective group discussions.

While the conversations often involved many people, only a single person could "drive" (e.g. hold the mouse). Switching drivers was time consuming because the driver needs to sit at the console. Participants were forced to "back-seat drive" by describing desired viewpoint changes to the driver, but this was rarely satisfying. Additionally, it was often difficult for the person using the mouse to change the view effectively or move the pointer to the appropriate position because of the configuration of the space. These problems were compounded by the fact that the mouse pointer was only displayed on 1 of the 2 stereo viewpoints.

Because of the limitations of the mouse pointer, it was common for participants to attempt to point out parts of the molecule they were studying with their hands. While in some domains this would work quite well, the use of stereo viewing caused a great deal of confusion when participants used their hands for pointing(due to parallax). Figure 2 shows an example of this problem.

Because there was no explicit support for switching between multiple viewpoints and selection sets, participants spent considerable time recreating previous configurations.

The system's interface presented users with reasonable access to an immense set of operations. However, it did not necessarily make the operations most common in discussion readily available.

3.4 Functional Requirements

In addition to potential areas for improvement our collaborators had key requirements for the system. These were: full compatibility with PyMOL including access to all functions provided by PyMOL during a collaborative session and the ability to load PyMOL session files; and the system must be comfortably usable by groups of 3-6 people.

4 Design

After performing the task analysis we designed a collaborative molecular visualization system around the shortcomings, key tasks, and functional requirements we observed. This section presents the design decisions we made and the rationale behind those decisions.

4.1 Design Process

In order to make our system as accessible as possible to small groups of domain scientists we wanted to use primarily inexpensive, consumer level hardware for our system. We used this constraint as the basis for our design decisions.

Within the framework of this constraint we made a set of design choices that addressed the requirements found in our task analysis. The primary design choices we made were the input methods and hardware to use and the types of displays to support. We based these decisions on how we could best support our requirements given the constraint of using low cost consumer level hardware.

4.2 Input Methods

The collaborative interaction with the molecular visualization is the area where we felt we could make the largest improvement over existing practices.

Choice of Input Hardware Our input hardware must be able to support the key tasks we identified in a fashion equivalent to or better than using a mouse and keyboard in a single user context and it must be readily available and inexpensive in the consumer marketplace. We examined a variety of input strategies including multiple mice and keyboard, individual displays and video game controllers. As we examined these we realized that the input device type with the most prior use in group settings at the consumer level is video game controllers due to their portability and ease of use in a single display group setting. One potential pitfall with using video game controllers is that they might not be as flexible as a keyboard and mouse or individual touch screen setup. Because of this it was important to determine whether or not they could support our key tasks of view manipulation and pointing as well as a few other specific tasks. We found that video game controllers were excellent at supporting the core interaction metaphors of pointing and view selection and that the other key operations were limited enough that they could be mapped to buttons.

We chose to abstract our control scheme in order to be able to experiment with both Wiimote style controllers and dual stick controllers because both these controller styles are able to support view manipulation and pointing as core interaction metaphors and they have enough buttons to support the other important tasks. This abstraction also allows us to rapidly support a new game controller or change what control maps to what task.

Mapping of Functionality to Input Hardware Our system must support the key tasks in a way that is easy to learn and consistent. We chose to use bimanual input to separate view control and pointing/selection tasks and map other important operations to buttons on the controllers. Using the dominant hand for precision pointing and selection and the non-dominant hand for viewpoint control is a well established input metaphor[11, 12] and increases task performance and depth perception. This input metaphor maps well to video game controllers and is intuitive. Other important but less frequent operations are mapped to buttons. For operations that exist in multiple contexts such as selection and deletion we used consistent mappings. We used symmetric pairs of buttons such as d-pads for symmetric operations such as navigating a list of selections or changing the visualization style of a selection.

Cursor and Pointing Users must be able to clearly communicate what sub portion of the molecule they are referring to and effectively select residues, atoms and chains. We found attempting to point at a particular part of the molecule using ones hands in a single stereo wall context was often very confusing due to parallax issues. This led us to the conclusion that rather than relying on users to physically point using their hands and arms it was necessary to give each user a pointer inside the system.

While we could have used a variety of 3D selection and manipulation techniques as discussed in Bowman et al.[13], we chose to use a virtual pointer because this most closely resembled the existing selection metaphor of PyMOL. Figure 3 shows the pointer

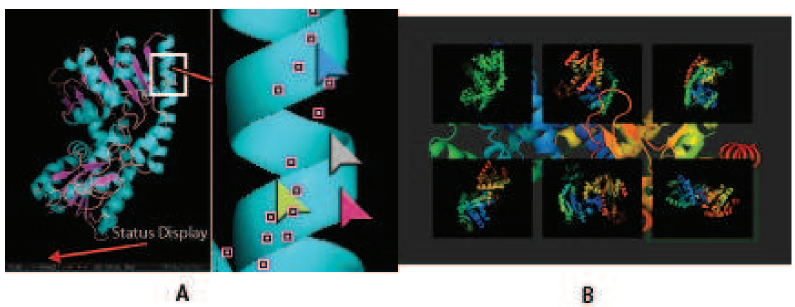

Fig. 3. A) Each user controls their own pointer which is used for both pointing and selection tasks. The active user is displayed at the bottom of the screen. B)Users can easily return to previously saved viewpoints by navigating saved graphical representations.

4.3 Display Type

Our collaborators felt strongly that stereo viewing was a necessary component to their collaborative discussions. For this reason we chose to support consumer level projectors and 3D HDTVs with stereo viewing capabilities. In the past this requirement would have required the use of expensive, custom hardware but consumer 3D devices have vastly improved in recent years.

4.4 View and Selection Bookmarking

In our task analysis we discovered that participants spent a great deal of time recreating previous views or trying to compare views. We chose to make view saving and loading easily accessible via the game controller Snapshots of views as a guide for selecting previously saved views. This functionality is available in PyMOL's desktop interface, but is obscure and requires typing function names using the keyboard. We felt it should be more prominent for collaborative visualization.

We also observed that participants frequently used different sets of selections to make comparisons or change visualization options. For this reason we made saving and storing selections easily accesible.

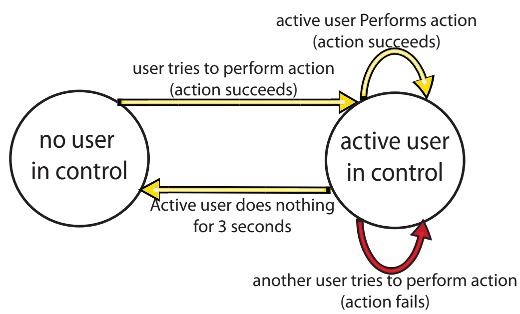

Fig. 4. The system only allows one user at a time to give input, other than moving their pointer. If the active user stops providing input for 3 seconds the system allows another user to take control.

4.5 Floor Control

Giving every user their own input device has significant advantages but it also has the potential for conflicting input. Our floor control policy attempts to prevent conflicting access without requiring explicit coordination. The model uses two states, as shown in Figure 4. In one state, anyone may take control by beginning an action such as viewpoint control. Once a user has taken control, they have exclusive control while they complete their action, and for a brief period afterwards to allow them to start a new action (to accommodate pauses). The state of floor control is shown in the display so that each user knows when they are in control or another user is in control in order to avoid confusion.

5 Implementation Details

We implemented our design as a plugin to the PyMOL molecular visualization software because of our users need to access it's functionality. Our implementation differs slightly between Wiimote and dual stick style controllers. These differences are discussed here.

5.1 Viewpoint Control and Viewpoint Selection

For both input devices we implemented rotation using the left thumbstick because in the bimanual import metaphor the non dominant hand controls the view and the dominant hand points. We made rotation the default control for the left analog stick and used the left trigger and bumper(easily pressed with fingers on the left hand) toggle panning and zoom of the view. In both cases we mapped saving views and loading from a set of saved views to one of the easily accessible buttons. Figure 3 shows an example of the viewpoint selection screen.

5.2 Pointing and Selection

Pointing on the Wiimote used a laser pointer metaphor: spatial tracking (using the controller's built in camera) allowed a user to point at the screen. On the dual stick style controller pointing was implemented by using the right analog stick[2] to make relative motion. In both cases selection uses the trigger on the right hand.

Figure 3 shows an example of several pointers being used at once. While the laser pointer metaphor seemed attractive, it proved ineffective for several reasons. There were challenges in making pointing stable and precise enough for the task. These issues we addressed through Kalman filtering [14] and using snapping to nearby objects. A practical issue, that the Wiimote's camera does not have sufficient field of view to work effectively with the large screen display, ultimately precluded us deploying the Wiimote solution. Our pilot studies also suggested other issues, particularly fatigue, as the user needs to hold the pointer up to maintain its position.

6 User Study

In order to evaluate our design we performed a user study on groups of experts in the domains of structural biology and related fields. These participants were either graduate students or professors in structural biology related fields. The goal of our user study was to both validate the individual elements of our design as well as the hypotheses that a molecular visualization system designed with multiple users in mind will facilitate more effective collaborative discussions than one that was designed for a single desktop user and that such a system is achievable using consumer level inexpensive hardware.

We used XBox 360 controllers in the user study because they seemed to be the most comfortable of the dual stick controllers, and support multiple wireless controllers simultaneously and because our pilot study revealed the wiimotes were not adequate for the pointing task. Our pilot study also revealed that with small groups the main purpose of floor control should be to disallow actual simultaneous input.

[2] The poor support for left handed users is a common criticism of dual stick devices. However, their widespread adoption in the marketplace suggests this may not be significant.

6.1 Methods

We performed an observational study on small groups of structural biologists and their collaborators. We observed 4 small groups of domain experts using our system in a collaborative discussion. Each session lasted 45 minutes and used a combination of fly on the wall observation, and a semi-structured interview afterwards. We gave each group a short tutorial on how to use the system and then encouraged them to discuss their work with each other using the system. Participants discussed protein molecules of interest to them without our intervention. Both the controllers and the mouse and keyboard interface were available. Afterwards we performed a semi-structured interview about their impressions of the system. We used video recording to analyze how the groups used the system and record answers to the interview.

We evaluated the individual elements of our design by whether the participants were able to complete key tasks efficiently using our interface and whether or not they felt they could complete those tasks with the same ease as with the mouse. We evaluated this both in terms of whether or not participants could complete key tasks either immediately, by the end of the tutorial, by the end of the group discussion or not at all; and based on the semi-structured interview.

We evaluated the overall effectiveness of our system based on how the participants use the system during the group discussion of a molecule and on the reaction in the semi-structured interview. We tested whether or not participants were able to use our interface to perform key tasks or if they resorted to using the mouse, and we measured how much of the time in the discussion was spent performing tasks that we had not mapped to the controller and whether they encountered significant bottlenecks similar to those observed in the task analysis. While the depth of the PyMOL molecular visualization system means that some tasks will necessarily be performed using the mouse and keyboard, a successful collaborative system should enable the vast majority of interaction with the system over the course of a discussion with the collaborative interface.

6.2 Results

In all cases, participants were able to quickly learn to use the game controllers for view manipulation, pointing and selection tasks. The overall response to the system was very positive and the group discussions were able to use the controllers for the overwhelming majority of desired tasks.

View Manipulation Twelve out of the 13 participants were immediately comfortable manipulating the view and the remaining participant was comfortable after the tutorial. Several participants felt that the view manipulation was easier than the mouse. 2 participants who were expert PyMOL users noted that while manipulating the view with the controller was easy and effective they were able to go faster with the mouse. Throughout all the group discussions no participant felt the need to use the mouse for view manipulation.

Pointing and Selection All participants were immediately able to use the pointer. 11 out of 13 participants found selection easy and the other 2 participants required time to adjust to the sensitivity. Several participants expressed appreciation of the improved clarity associated with the pointer compared to using hand gestures to point at specific pieces of the molecule.

View and Selection Bookmarking Participants were immediately able to use the view and selection bookmarking system after being shown how to use it. Over the course of the evaluation these functions were not used very much during the group discussions. We speculate this functionality is new to most users, as it is typically inconvenient and therefore infrequently used on the desktop. Several participants were interested in using pre-prepared selections as opposed to new selections which we plan to add support for in the future.

Floor Control Disallowing simultaneous input and displaying the active user proved adequate for the group sizes we used to test the system.

Overall Effectiveness Participants only used the mouse and keyboard to achieve unusual tasks that were not mapped to the controller. The vast majority of the time spent interacting with the system was done through the controllers. In all group discussions more than 90 percent of the time spent interacting with the visualization was done via the controllers. The bottlenecks to discussion we identified in our task analysis did not slow down the discussions.

All of the participants felt that the collaborative interface was better than the desktop interface for the majority of uses in a collaborative session. Some felt that we should have included a way to toggle ligand(small molecules that bind to the protein) display. We felt that this demonstrates that they preferred the controller to the mouse and we plan to include this functionality in the future.

6.3 Analysis of Results

We found that a visualization system designed with multiple users in mind will be more effective for group discussions than simply displaying a single user system on a large wall. Additionally we demonstrated that this can be achieved at a hardware cost similar to a medium-end home entertainment system as we were able to use consumer level displays and inexpensive video game controllers as input devices.

Our design succeeded in all areas. In the area of bookmarking we discovered improvements that will be incorporated into the next iteration of the design.

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