

# Designing interaction with molecule visualizations on a multi-touch table

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## ABSTRACT

Molecular visualizations are an important tool in modern day biology research. This literature study describes the first step in the process of moving molecule visualizations from desktop computers to multi-touch tables. To control these 2D visualizations of 3D objects on a multi-touch table, a set of gestures has to be defined. Since there is little research about controlling 3D objects on a multi-touch table, several state of the art gestures are examined to see if they are suitable to be used in molecule visualizations. The results show that not every interaction needs to be a multi-touch gesture, and that a user test is needed to confirm if the chosen gesture set is suited for users unfamiliar with multi-touch interaction.

## Keywords

Bioinformatics, molecule visualization, multi-touch table interaction, BioRange, direct-touch interactive tabletop surfaces

## 1. INTRODUCTION

In modern day research, biologists analyze the molecular structures of proteins to find out valuable information about the causes and workings of diseases. The researchers of the BioRange@UT project [1] want to enable biologists to analyze visualizations of these molecules using a multi-touch table. Multi-touch tables provide a better environment for viewing molecules with multiple persons, as well as on a larger scale. This makes the multi-touch table a more suitable visualization tool than an ordinary desktop system. Another downside of using a desktop is that controlling a molecule visualization with just a mouse is not quite as intuitive as you might want. The multi-touch table can provide a solution for this by enabling visualization control with two hands.

In this paper a literature study is reported that examines the interaction possibilities with molecule visualizations. Based on the tasks that biologists perform with molecule visualizations, existing multi-touch interactions are analyzed to determine whether they remain effective when used with molecule visualizations.

## 2. RESEARCH QUESTIONS

The goal of the research is to answer the following question:

*Can current (multi-)touch screen interactions be used by biologists to effectively interact with molecule visualizations on a multi-touch table?*

The term *effective* in the main question means that the interactions are easy to learn, easy to use and most importantly: they should be optimal for achieving the interactions the biologists want to have with the table. The main question will be answered using the following sub questions:

1. What is the state of the art in interaction with multi-touch tables and other touch screens?
2. Are there existing interaction designs for molecule visualizations or other 3D objects?
3. Which tasks do biologists perform when analyzing molecule visualizations?
4. How can the existing interactions on multi-touch tables be used to perform these tasks?

## 3. RESEARCH APPROACH

The first two sub questions are answered using a literature study. The state of the art in multi-touch interaction is described in section 7. The only paper about interaction design found for the second sub question is a paper by van Liere et al. [20]. Because this interaction design has no relation to multi-touch interaction, this paper is discussed in the further research section. With some emulation though, existing visualization applications can be used on a multi-touch table. More about this solution is described at the end of this section.

In order to determine which interactions with molecules are required, we need to know what biologists actually want to do with the molecules (sub question three). This is again answered by a literature study.

The state of the art interaction solutions can be matched with the actions of the biologists in order to answer the last sub question. The result of this matching is a table in which the different alternatives are lined up with their strong and weak points. With this, the main research question is answered.

As a focus for future implementation Jmol [2] is used, in combination with the DiamondTouch table [3]. Jmol is an open source Java tool for displaying and measuring molecules. Because its API is known and it is built in Java, it can be easily adapted or expanded. However, Jmol cannot perform basic operations such as translation and zooming using only the mouse. This can be done by Yasara [4], which offers similar functionality in a closed source environment. Because Yasara can be operated with just a mouse, it can be emulated on the multi-touch table using software from the table

designers. This emulation means that the mouse cursor can be controlled by tapping and dragging on the table. Tapping with one finger is a left click, tapping with a second finger besides a first finger already on the table emulates a right click. The middle mouse button is not emulated, which means that the translation gesture in Yasara cannot be analyzed. By using Yasara as a standin for Jmol, the state of the art solutions have a real molecule visualization tool to compare to.

## 4. RELATED WORK

There is virtually no research into interactions with molecule visualizations. Van Liere et al. [20] have researched how depth cues should be used to support the studying of 3D molecules. They test their solutions on two systems that both use eye tracking and object tracking to control the molecule. The user holds a small cube that is tracked to rotate the molecule on the screen. Using a pen that is also tracked, the user can select or trace parts of the molecules. To increase the 3D experience, the eyes of the user are tracked so the user can really look around an object.

The developers of the DiamondTouch table at the Mitsubishi Electric Research Laboratories (MERL)[3] have published a number of papers about their table, usually in collaboration with others. For instance, they have published papers about the design of multi-touch tables [17] and about observations and experiences with the use of the table [15]. Yet another paper studies performance differences between direct-touch and mouse input with both one-handed and two-handed tasks [6].

A study by Moscovich and Hughes compares one-handed and two-handed gestures while performing tasks on 2D objects, such as aligning and docking. The core of their study is a kinematic analysis that determines the amount of control and the constraints that are present in the freedom your fingers give you.

Another aspect of multi-touch tables is the fact that multiple people can access the table at once. A number of studies have investigated the behaviour of people in these situations. Tse et al. [19] have written about interaction between two people that work on the same table, while playing speech-augmented games. Grossman and Balakrishnan [7] have studied collaborative work on a volumetric (real 3D) display. Scott et al. [16] have investigated territorial behaviour of people on a multi-touch table, and how software can use this behaviour for accessibility and cooperability.

## 5. USER PROFILE

Kulyk and Wassink [10] have done a study to see what types of users there are in the field of bioinformatics. Real bioinformaticians (domain experts) are experienced in the use of existing molecule visualization tools. The other type is the novice user. These users are often biologists or other scientists with limited computer experience. Anecdotal evidence suggests that biologists do not use molecule visualization tools yet, so the research is aimed at bioinformaticians. The bioinformaticians can play an important role in multi-disciplinary teams, as they can assist biologists by explaining the molecule visualizations.

## 6. USER ACTIONS

What does a user want to do with the molecule visualizations? By analyzing studies by Vyas et al. [21] and Kulyk

and Wassink [10], the following basic actions can be distilled:

- Translation
- Rotating (around the center of the molecule)
- Zooming
- Selecting groups/atoms
- Changing display modes

These actions are easily achievable in most molecule visualization programs such as Jmol [2], Yasara [4] and VMD [22]. Rotation is a difficult action to define. It is not quite clear if rotation along the X and Y axes is enough, or if the Z axis should be added as well. Yasara can perform rotation along the Z axis as well as X and Y, but only using key bindings. With the mouse, only rotation along the X and Y axes can be achieved. When judging the state of the art gestures, a solution will not be punished for rotation along just two axes.

Molecule visualization software typically uses cartoon views of molecules. The ball-and-stick view is most common, which shows coloured balls for atoms and sticks for the bonds between them. If you want to see the real volume of the molecule (which is larger than the balls and sticks), the van der Waals surface can be toggled. These are examples of display modes that should be accessible to the users. Changing the current display mode is not easily achieved by implementing a single gesture. This action will need a context menu. A context menu can be called by a gesture, or it can simply appear somewhere around the edge of the screen. This gesture is not included in the comparison table. The gesture that is most used when studying molecules is the rotation gesture. The zooming and translation gestures are less important, since the molecule is automatically displayed in the center of the large multi-touch table. Selection and display mode changing have the lowest priorities. These priorities are important, because they should be the deciding factor when two gestures interfere.

## 7. STATE OF THE ART

When describing and comparing the state of the art gesture solutions, a number of frequently used terms are used that are close together in meaning. A gesture is called *intuitive* if it is the first gesture a user would make if he wants to perform the corresponding action, such as selecting something by pointing at it on the table. *Natural* gestures are gestures that resemble actions in the real world. For instance, if you want to rotate a glass on a table, you make a twisting gesture. A gesture is *easy to learn* if it is not intuitive, but can be learned quickly after explanation. A complex gesture requires a large number of contact points or complicated movements to perform.

### 7.1 Yasara

#### 7.1.1 Description

Yasara [4] can be controlled using the mouse, or on a multi-touch table with emulation as was shown in section 3. Translation is done with the middle mouse button. Unfortunately, this button is not emulated by the multi-touch software. Rotation is done using the left mouse button. By holding the

button (or touching the table) and dragging, the molecule is rotated. Moving left and right controls Y axis rotation, moving up and down controls the X rotation. Dragging at an angle rotates two axes at once. No Z rotation is possible with the mouse controls. Zooming is done by holding the right mouse button (or touching the table with two fingers) and dragging away from the originating point. By dragging up or right, the molecule is zoomed out. Down or left dragging zooms in. Selection is done by simply clicking the left mouse button (tapping with one finger).

### 7.1.2 Evaluation

The rotation gesture is very easy to learn. Despite the fact that it can only rotate the molecule around just the X and Y axes, the user can still view all sides of the molecule without complicated gestures. The zooming gesture feels a little strange on a multi-touch table, because of the awkward mouse emulation. A two-handed gesture would be better for zooming. The selection gesture is the easiest and most intuitive of all, and does exactly what probably every user would expect.

## 7.2 Multimodal tabletop gaming, Tse et al.

### 7.2.1 Description

Tse, Shen, Greenberg and Forlines [18, 5] have developed a way of interacting with games through the use of both gestures and speech. They have made multi-touch interfaces for The Sims, Warcraft 3 and Google Earth. The gestures they designed are not only supposed to control the game, they also show other users/viewers of the table what is happening. The speech interface is used to enhance the gestures, such as "Attack here [point]". As gestures are the main focus for this research, the speech actions are not taken into account.

The gesture controls for The Sims are the easiest. Grabbing an object is done by placing all five fingers on the object (pinching). The user can then slide the object over the table, and drop it simply by releasing his fingers off the table. The second gesture is the stamp, in which the user places his fist on the table to place an object selected from the user interface,

The Warcraft 3 gestures are a little more complicated. Sliding a flat hand across the table pans the map around. Pointing at a location with one finger selects units or locations. Pointing with two fingers triggers a context sensitive action, such as attacking or moving. Selecting multiple units in an area is done using the sides of two hands, the way you would pick up a box.

Google Earth is the most interesting application, because it can zoom and has a 3D level. Panning is done by sliding a finger over the table. Double tapping a finger results in a 2x zoom at that location. Spreading two fingers apart or together results in zooming out and in respectively. If these actions are done rapidly, the zoom continues until the fingers are released. Sliding with one hand tilts the 3D view to street level (flat), while the five-finger pinch tilts the 3D view to top view. The two-finger zooming gesture seems quite intuitive, though the 3D view controls are not.

### 7.2.2 Evaluation

The controls for The Sims are only suited when the visualization has to be translated, for instance in case of very large molecules. The five-finger pinch is quite a natural gesture to do pick up a tree in the Sims, though it is not so natural for translating large molecules.

The Warcraft interactions are more suitable, because it handles (multiple) selection and panning. The panning gesture can be used as translation gesture when dealing with molecules. Zooming is not featured, but that can be added. The zooming and panning (translation) gestures in the Google Earth application seem quite adequate for use in molecule visualizations. The only thing missing is a description of the rotation gesture, although that is a rotation around just one axis. The 3D view controls that are not intuitive will not have to be used at all.

Nearly all gestures proposed by Tse et al. appear to be easy to learn, apart from the 3D view controls in Google Earth. Though it has to be said that this is probably a more complex 3D environment to control than a the molecule visualization. In Google Earth the camera has to be able to view the entire world around it, while being able to sweep from street level to birdseye view at the same time. A visualization tool only has to be able to view one object from all sides.

## 7.3 Shallow-depth 3D interaction, Hancock et al.

### 7.3.1 Description

Hancock, Carpendale and Cockburn [8] tried to imitate real desktop behaviour by implementing shallow-depth gesture interactions with a multi-touch table. Shallow-depth means that the interaction is in 3D, but with extremely limited z depth. In their study they designed interactions with a small 3D cube using one, two or three points of input. Using these interactions the cube is translated along the x and y axis, and rotated along the x, y and z axis. No zooming is done. Test results show that the one- and two-finger interactions are the hardest to use, so I will only consider the three-finger interaction. The first point of contact is always the point that is used to translate the cube and to serve as locking point for rotation. The second point of contact is responsible for rotation along the z axis. The final contact point enables rotation along both the x and the y axis.

### 7.3.2 Evaluation

Because the molecule visualizations do not have to be translated and rotated in the same gesture, the first point of contact can be omitted from the interaction. The reference point for rotation is already defined as the center of the molecule. This reduces the complexity and gesture freedom as only two points of contact are required. Two contact points can be fingers of both hands, on any place of the table. Experimentation is required to find out if this interaction style is easy to learn for users. A problem with this interaction is that there is no zooming possible, unless a new gesture is implemented.

## 7.4 Rotation and translation mechanisms, Hancock et al.

### 7.4.1 Description

Another study by Hancock [9] (along with Vernier, Wigdor, Carpendale and Shen) is about a number of mechanisms to rotate and translate a 2D object on a surface.

The first and easiest of the mechanisms is by explicit specification. With a number of sliders or dials, the position and orientation of the on-screen object can be specified. This does not include gestures other than moving a slider, but the meaning of the controls is immediately clear.

Independent translation and rotation are the easiest gesture based mechanisms. To translate the object, simply touch and drag the object. The same touch and drag gesture is used for rotating. When dragged the object will rotate along the angle between the first point of contact, the center of the object and the point of release.

The other mechanisms described combine rotation and translation in one gesture. These mechanisms are more suited for passing objects around on a multi-touch table, something that will not have to be done in this research since only one molecule is displayed on the table.

#### 7.4.2 Evaluation

The explicit specification is perhaps the easiest way of controlling an object, if the user has no experience with gestures. The presence of a control widget makes it intuitive for the user to direct his attention and gestures there. It is also easily expandable to accommodate zooming and rotation along more than one axis. This mechanism is also useful for easily storing and recalling specific positions and orientations. The main disadvantage is that the user cannot control a 3D object in a natural manner, because the gestures are not made on the object itself. Furthermore, the sliders/dials should be usable for any user from any position around the table. This may be achieved by tracking where all users stand around the table.

Independent rotation is a good way of rotating a 2D object, but rotation along more than one axis is problematic. The idea of independent rotation and translation is good though. This can easily be achieved by changing the translation gesture from a single finger point to a five finger pinch or flat hand gesture.

### 7.5 Rubbing and tapping, Olwal et al.

#### 7.5.1 Description

Olwal, Feiner and Heyman [14] have investigated the use of rubbing and tapping techniques to perform precise selection on single-touch displays. The rubbing and tapping gestures are used to zoom in on the interface during the selection process. These two novel techniques are compared to traditional methods Take-Off and Zoom-pointing. Take-Off lets the user control a cursor that is projected just above the tip of the finger, to avoid occlusion of the object to be selected. Zoom-pointing is done by selecting zoom mode using a button, dragging a box area to zoom, and pointing to the object to be selected.

A user study showed that rubbing techniques are inconvenient when performed on a resistant surface. The techniques that zoom in by tapping are very fast and precise in selection. Zoom-pointing, despite being slow, is quite intuitive for most users. Take-Off is clearly not preferred by most users

#### 7.5.2 Evaluation

Precise selection is not a big issue when projecting molecules on a large display. Zooming is useful, but high speeds are not required. Tapping the screen to zoom can be a good solution, because it is easy to remember and fast to do. Zoom-pointing is a better option, because the user can specify exactly which area he wants to enhance. A problem with Zoom-pointing is the requirement of a button to select or reset the zoom mode. This is not suited for a large display that can be accessed from all sides.

### 7.6 Visual Touchpad, Malik & Laszlo

#### 7.6.1 Description

Malik and Laszlo [12] have built a system that can track the actions and postures of a user's hand on flat surfaces. In essence this is not a touch screen, but the gestures are also suited for that purpose. In a simple picture manipulation application users can translate, rotate and zoom both the pictures and the entire view. Both one-handed and two-handed interactions are described.

One-handed object manipulation is done using tapping for selection, dragging for translation and finger orientation for rotation. Finger orientation cannot be realized on a multi-touch table, so this gesture cannot be made. There is no zooming gesture in this gesture set.

To manipulate the view using one-handed gestures, the user has to pinch his index finger and thumb on the screen. The focus point becomes the center between those two fingers. Moving the entire hand makes the view translate. By twisting the hand, the view can be rotated. If the fingers end up in an awkward pose, the gesture can simply be released and remade in a comfortable pose (like operating a screw driver). By moving the two fingers further apart or together, the view can be zoomed.

The two-handed gesture set is copied from Kurtenbach et al. [11]: two-handed stretchies. This technique lets the user select two points on the screen using two fingers. These two points remain under the fingers at all times. By moving the fingers, the object or screen can be translated, zoomed, and rotated along one axis.

To accommodate additional functionality such as drawing or coloring, Malik and Laszlo have implemented a pie menu. This menu with options spread around in a circle can be accessed using the non-dominant hand. The menu appears around the finger of this hand for example when double tapping the screen. The non-dominant hand can then select a mode or option, while the dominant hand can make a drawing for instance.

#### 7.6.2 Evaluation

Selecting gestures from the different sets, one combined gesture set can be made. The selection and dragging gestures in the one-handed object manipulation are commonly used, so those can be safely adopted. To rotate and zoom a molecule, the options of the view manipulation could be used. They appear to be quite easy to use, though only for small adjustments to the view/molecule. The larger the adjustments become, the more you have to redo the gestures. Another thing to note is that using these gestures, users will not be directly controlling the molecule, making it a less natural interaction for a multi-touch environment.

The pie menu is a great tool for performing additional actions. This can be used for instance to select a measuring tool, or to change the display mode of the molecule.

## 7.7 3D Manipulation, Moscovich

### 7.7.1 Description

In his PhD thesis [13], Moscovich acknowledges the fact that the step from 2D to 3D manipulation is a large one. Ideally, he wants to achieve rotation and translation of a 3D object in one fluid motion, using only three points of contact. For both rotation and translation, only two fingers are needed. The third point of contact is reserved to be used as mode switcher between the two. Rotation around the X and Y axis is achieved by the same movements on the 2D surface, while Z axis rotation can be done by twisting the two fingers around their combined center (centroid). Moscovich does not use a zooming mechanism, but a similar effect is created by translating the object along the Z axis.

### 7.7.2 Evaluation

Moscovich's gesture set is not described in too much detail, so it leaves a lot to the imagination. The rotation mechanism appears to be easily learnable, although novice users might have problems with it. Translation seems somewhat complex, because Z axis translation (alternative zooming) is included.

## 8. RESULTS

For convenience, the strong and weak points for the actions in the different solutions have been summarized in Table 1. All that remains is to select which gestures are best suited for the various actions.

The most important gesture is the rotation gesture. The three axis rotation gesture by Moscovich seems the best solution for advanced users. The gesture can be started anywhere on the table, which makes it more natural than the widget solutions. This gesture might be the best option from a multi-touch point of view, though it will take some time to master for novice the users. These users will probably prefer the gesture as it exists in Yasara/Jmol. This gesture is clearly the simplest gesture available for multi-axis rotation.

The widget rotation solutions also appear very user friendly. The problem with them is that the user is not touching the molecule itself but a device, similar to a keyboard that controls on-screen action. In this category, the explicit specification using sliders is the best option. Even so, I think that users will prefer the Yasara rotation gesture over the sliders. The easiest translation gesture is of course to drag the molecule with a finger. This gesture would interfere with the Yasara rotation gesture, so another more complex gesture should be chosen. A good candidate I think is the panning gesture from Tse's adaptations of Warcraft 3. by using a flat hand to move the molecule, the user has a natural, easy to learn gesture that is clearly distinguishable from the one-finger drag.

For zooming, the gesture by Tse in Google Earth seems the best choice. By spreading and closing to fingers, the user has a natural zooming gesture. The gesture can be used with one or two hands, whatever suits the user best. Alternatively, the tapping solution or the explicit specification slider can be used to control zooming. These gestures are less natural though.

For selection only one real solution can be given: the one-finger point. This solution is the first thing people try, and is used everywhere.

To change display modes, some sort of context menu is desirable. Though this action is not included in the results table, there is a solution that addresses this problem. The Visual Touchpad by Malik and Laszlo suggests using a pie menu, that can be called to appear around a finger for instance. Calling this menu can be done by double tapping the screen for instance, perhaps accompanied by a point from the other hand. In the pie menu different options can be included. Possible menu options could be van der Waals surface display or molecule orientation memory.

I think the resulting gesture set is a good answer to the main research question. From the information available in the literature, it appears that the gesture set allows for effective interaction with molecule visualizations. Further research in the form of a user test is needed to confirm these ideas.

## 9. CONCLUSIONS

This paper described how existing gestures in (multi-)touch interaction can be used to control molecule visualizations. The results show that a multi-touch gesture is not always suited to perform an action. The rotation gesture is the most important gesture for molecule visualizations, so this gesture should be easy to make. Multiple contact points can be used to rotate, but a single finger gesture is much easier to understand and operate. On the other hand, gestures should be natural as well. Zooming for instance is natural when it is done by moving fingers away or towards each other, instead of using a single finger drag in existing visualization software. To conclude, the gesture set described in section 8 is a set that should be easy to learn and use by the users of the software. It is not capable of very complex interface manipulation, but that is more of a requirement for computer aided design applications.

## 10. FUTURE WORK

An obvious direction for future work is to implement a gesture interface for Jmol. With this, the gesture set can be tested for efficiency and possibly adapted. It is then also possible to see which mode of rotation (two or three axes) is best for the users, and how they want to control it (number of contact points). Additional or alternative gestures can also be designed and tested. Instead of zooming with two fingers, some users might want to zoom with two flat hands. This example of an additional gesture can be used to make the gesture set more robust, flattening the learning curve. Another interesting point is to study how the users act when analyzing molecules together. Does the application need some sort of turn-taking mechanism? How can multiple people do things at the same time without disturbing the operations of others? All these topics have been researched before (see section 4), but those studies are about controlling multiple objects on a collaborative interface instead of a single 3D object.

The system could also be expanded to make a connection with other relevant information, such as extra information about molecules in text. Can this be added to the display on the multi-touch table? What are the limitations and possibilities of text when there are multiple people around the table wanting to read it?

Solution	Translation	Rotation	Zooming	Selecting
Yasara Krieger		+ Easy to learn + Full control with two axes	+ Easy to learn - Unnatural	+ Intuitive
Multimodal tabletop gaming Tse et al.: The Sims	+ Easy to learn			+ Intuitive
Multimodal tabletop gaming Tse et al.: Warcraft 3	+ Easy to learn + Natural			+ Intuitive
Multimodal tabletop gaming Tse et al.: Google Earth	+ Easy to learn + Natural	- Only Z axis	+ Intuitive + Natural	
Shallow-depth 3D interaction Hancock et al.		+ Rotation around 2 or 3 axes possible		+ Intuitive
Explicit specification Hancock et al.	+ Intuitive - Unnatural	+ Intuitive - Unnatural	+ Intuitive - Unnatural	
Independent rotation Hancock et al.		+ Easy to learn - Only Z axis		
Rubbing and tapping Olwal et al.: Tapping			+ Fast + Easy to learn	
Rubbing and tapping Olwal et al.: Zoom-pointing			+ Precise + Easy to learn - Requires widgets	
Visual Touchpad Malik & Laszlo	+ Easy to learn	- Unnatural - Only works well around one axis	+ Natural	+ Intuitive
3D manipulation Moscovich	- Complex	+ Rotation around three axes possible	- Combined with translation	

**Table 1: Solutions mapped to actions. If a cell is empty, the solution has no gesture for that action. An explanation of the terms used in the table can be found in the introduction of section 7.**

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