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METHODS FOR INVESTIGATING STUDENTS' LEARNING AND INTERACTION WITH A HAPTIC VIRTUAL BIOMOLECULAR MODEL

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Abstract

Although immersive haptic virtual technologies are emerging rapidly in modern education, few methods exist for delivering data on the pedagogical merits of such models in the molecular life sciences. This paper reports on a selection of methods that we have used to obtain and analyse data on students' learning and interaction with a haptic virtual model of protein-ligand docking, previously designed by author PBP. The methods have been developed and employed in a university setting where the model has been used during advanced biomolecular interactions courses. In this regard, we present data-collection methods that include written items, interviews, think-aloud tasks and automated time-stamped logs, and corresponding quantitative and qualitative analytical procedures such as pre/posttest comparisons, word usage analysis, and visualized profiling of students' interaction with the model. Our results suggest that these methods are useful for generating valuable information on students' learning gain, changes in conceptual understanding, reasoning processes and patterns of interaction with the model. Dissemination of such methods could provide an empirical contribution to the dearth of research instruments in this domain. Future research will develop these methodologies to explore the relationship between using the model and students' conceptual and embodied learning.

Introduction

Other than perceiving information visually and aurally, recent virtual environments (e.g. Reiner, 2004) engage a user's haptic sense, which is the perception of touch and force stimuli such as texture, hardness and shape (Lederman & Klatzky, 1987). The haptic modality integrates kinaesthetic and cutaneous sensory input, allowing for exploration of the immediate surroundings through active touch (Klatzky & Lederman, 2002). Haptic experiences have been exploited in human-computer interaction technology so that users can feel and manipulate virtual objects that exist in 3D space (e.g. Srinivasan & Basdogan, 1997). While such environments show great promise for education, little science education research has considered students' learning and interaction with haptic virtual models (Minogue & Jones, 2006). Furthermore, work on haptic virtual models in the molecular life sciences has largely concerned usability and evaluative dimensions (e.g. Martin, Eid, & El Saddik, 2008) and hardly any empirical inquiry has focused on uncovering cognitive and learning aspects underlying users' interaction.

For the last five years, our group has been concerned with obtaining information on students' learning about biochemical interactions, and in particular, protein-ligand docking (e.g. Bivall Persson et al., 2007). The molecular processes of living systems are highly dependent on proteins and their capacity for molecular recognition, and it is thus of critical importance for students to understand the concept of docking. This pertains to the physical process during which a ligand molecule (often a relatively small molecule) and a protein in solution come into proximity of each other and interact favourably, eventually forming a complex in which the ligand binds to an area of the protein surface. Individual non-covalent intermolecular forces are transient in solution, but strong binding between a protein and a ligand is made possible by cooperative reinforcement of several simultaneous weak interactions. At a conceptual level, protein-ligand docking represents the intersection of at least three important perspectives of

molecular life science: the dynamic nature of biomolecular systems, the nature and geometric dependencies of non-covalent intermolecular interactions, and the importance of chemical and sterical constraints in systems involving macromolecules. With respect to the construction of these concepts, our group's work has been focused on investigating learning with a virtual haptic model developed by author PBP.

Rationale

Description of the haptic virtual protein-ligand docking model

The bimodal system developed by Bivall Persson et al. (2007) incorporates 3D stereo graphics and force feedback to represent the docking process. A haptic device is used to manipulate the ligand, while a simultaneous force output is delivered as the ligand is moved close to a protein (Figure 1, right). The force acting on the ligand, and correspondingly perceived by the user through the haptic sensory channel, is calculated by the system using the protein's potential field and the molecular structure of the ligand (see Bivall Persson et al., 2007). Thus, the force acting on the ligand during docking is determined by the local environment in the protein's potential field. This corresponds to the sum of the energetic potential field gradients for the ligand atoms, according to equation 1.

$$F_{ligand} = \sum_{i=0}^{n} -\nabla\phi_i(x_i) - q_i\nabla\phi_{esp}(x_i) \qquad (1)$$

Where n is the number of atoms in the ligand, i denotes each individual atom, and q_i is the charge on atom i. $\phi_i(x_i)$ is the potential field that is specific for the species of atom i, while $\phi_{esp}(x_i)$ is an electrostatic potential field. The force calculated from the potential field surrounding the protein is scaled to be perceptible by the human haptic sense, and presented to the user through the haptic device. Several docking systems that incorporate different protein types and corresponding ligands can be explored with the model, which can be visually rendered in several representational modes (e.g. Figure 1, left).

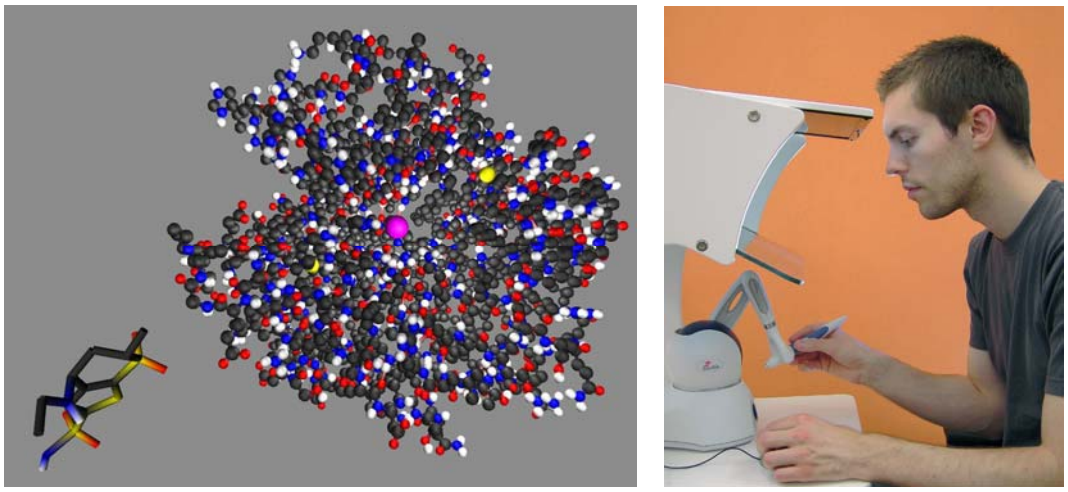

Figure 1. Left: Screenshot showing ligand (small molecule) and protein (large molecule) from one docking system. Right: Photograph of a student using the hardware that renders the haptic virtual model.

Research purpose

Although haptic technologies offer exciting pedagogical promise, few empirical methods exist for explicitly investigating students' learning and interaction with haptic virtual models in the molecular life sciences. The haptic virtual model described above has been used during advanced biomolecular interactions courses offered at Linköping University, Sweden, with classes ranging from 9 to 23 students. Generating any useful information concerning the benefits of such models in real educational contexts requires suitable data-gathering and analytical

methods to measure their role in learning and understanding. It is our opinion that this endeavour should involve obtaining a combination of 'before and after' as well as 'moment-by-moment' data. Based on this motivation, the purpose of this paper is to present a selection of methods that we have developed to respond to the following questions:

- How can students' learning outcomes be measured after interaction with the model?
- How can changes in understanding be identified and characterized?
- How can real-time interaction with the model be monitored?

Methods for Investigating Students' Learning and Interaction with the Model

How can students' learning outcomes be measured after interaction with the model?

In presenting examples of methods that have yielded empirical results, a selected written item that was used in two pre/posttest studies during separate years (termed study 1 and 2 in this paper) was as follows:

> *Describe the process of a substrate coming into and finally binding in the active site of an enzyme. Imagine that you are sitting on the substrate, describe everything that happens on the way in, until the substrate has bound.*

Student responses to this item were scored against a list of possible acceptable answers constructed by two biochemistry educators. Here, several important protein-ligand docking principles (e.g. complementary fit and intermolecular dynamics) were used to collate a set of scientific propositions that represented acceptable answers. Upon using this scoring scheme, the agreement between the assessors on students' responses to the above item was 85%, indicating a favourable inter-rater reliability. Any gain in learning after interacting with the model (with haptic feedback enabled or disabled) was measured by comparing students' pretest and posttest scores (Table 1).

Table 1. Comparison between students' pretest and posttest mean scores.

Group		Pretest (%)	Posttest (%)
Study 1 control	(haptic feedback disabled)	35	39
Study 1 treatment	(haptic feedback enabled)	39	54
Study 2 treatment	(haptic feedback enabled)	32	51

In addition to comparing students' pre/posttest scores, students' actual answers to the item could also be compared. For example, consider the following student's responses to the item during the pretest and posttest from study 2, respectively:

> Pretest: *The substrate approaches the active site, which is filled with water. The water is displaced and the substrate begins to enter the enzyme, which is not quite "rigid" but rather flexible, allowing the substrate to enter. Once inside, the substrate is repositioned to minimize repulsive interactions, and then it passes through a slow transition state and binds covalently to the enzyme.*
>
> Posttest: *As the substrate approaches the active site a few attractive interactions might be created. Although this might not be enough for it to be "sucked" into the protein immediately, it will be more difficult for it to diffuse away. After a while the ligand might find more interactions where the higher the number of attractive interactions the higher the probability of binding will be. The substrate uses "trial and error" to find its optimal position inside the protein, with the highest number of attractive, and the lowest number of repulsive interactions, until it has found the best possible position and is stuck there.*

Comparing these responses was used to shed light on this particular student's learning gain shown by the difference score. For instance, the responses indicate that this student might very well have learnt about aspects of the principle of complementary fit between protein and ligand, and associated attractive forces. In particular,

analysis of the posttest response reveals that the student has learnt about the role of attractive forces in docking, compared to the pretest response in which docking is described as a process of minimizing steric hindrance. Hence, this item was found to deliver both quantitative and qualitative information on students' learning outcomes after interacting with the model.

How can changes in understanding be identified and characterized?

Analysis of students' word usage from responses to the item is one way to investigate any changes in understanding. In particular, by considering the nature of the words that are expressed, the conceptual understanding attributed to docking can be gauged. Such analysis by Bivall Persson et al. (2007) has revealed several categories of reasoning about docking. Two reasoning categories are the chemical and force categories. Chemical reasoning is shown when students use words that describe chemical phenomena (e.g. 'acid', 'hydrophobic', 'polar'), while force reasoning consists of word usage that describes physical interactions between molecules (e.g. 'pulls', 'repels', 'attracts'). The same response from Study 2 presented in the previous section, is reproduced here, with **chemical** words in **boldface** and force words underlined:

> Pretest: *The **substrate** approaches the **active site**, which is filled with **water**. The **water** is displaced and the **substrate** begins to enter the **enzyme**, which is not quite "rigid" but rather flexible, allowing the **substrate** to enter. Once inside, the **substrate** is repositioned to minimize repulsive interactions, and then it passes through a slow **transition state** and binds **covalently** to the **enzyme**.*
>
> Posttest: *As the **substrate** approaches the **active site** a few attractive interactions might be created. Although this might not be enough for it to be "sucked" into the **protein** immediately, it will be more difficult for it to diffuse away. After a while the **ligand** might find more interactions where the higher the number of attractive interactions the higher the probability of binding will be. The **substrate** uses "trial and error" to find its optimal position inside the **protein**, with the highest number of attractive, and the lowest number of repulsive interactions, until it has found the best possible position and is stuck there.*

After interaction with the model, there is a two-fold increase in the frequency of the student's usage of force words, from 3% to 7% (of total word usage). Simultaneously, the frequency of chemical word usage decreases from 18% to 6%. This analysis allows for an observation of the types of, and shifts in, understanding constructed from engaging with the model.

In addition to word analysis, semi-structured interviews can be used to investigate conceptual understanding and reasoning about docking after interacting with the model. For example, consider the following student quotes obtained from interviews during study 1 and 2:

> *You know the chemistry… properties of different groups… different types of forces… What haptics did was to couple this together into a coherent whole.*
>
> *…you never really have a picture like that of how, it [docking] happens from the outside in, maybe into some cavity where it [ligand] is influenced by forces all the time, to actually find the correct position…*
>
> *...the ligand bumps around when I try to dock it. Is it really so random and dynamic? I thought it was more like a magnet, that the ligand was sucked into the binding site into one correct position...*

At least three potential changes in student understanding can be revealed from analyzing interview data. For example, in the case of the first quote, there is a distinct metacognitive dimension connected to the student's use of the model. In contrast, the student who delivers the second quote clearly adds knowledge about the influence of forces to his/her already existing conception of a 'correct' binding position. Lastly, as demonstrated by the third quote, interacting with the model might also induce a cognitive conflict with the consequence of a student challenging or replacing an existing conception. Hence, interview data can provide rich insight into the impact of the model on the current status and changes in students' conceptions of the docking process.

How can real-time interaction with the model be monitored?

In parallel with the data collection instruments described above, specific tasks were also designed to obtain information about students' interaction with the system. One such exercise consisted of the following:

> *Write a description of how you predict the ligand to dock. Now, try to dock the ligand in the way that you have predicted. During this exercise, try and express aloud what you are thinking about and experiencing. When you have found a docking position that you are satisfied with, press the save-button.*

The following verbal exchange is an excerpt taken from a think-aloud session based on the item above, delivered during a student's successful attempt to locate the correct docking site on a protein.

> Interviewer: *How are you currently experiencing the potential pit [Student previously described the binding site as a 'pit' of potential energy minimum]*
>
> Student: *Well, here [a region on protein surface] there is like a strong repulsion whereas here [makes whistle sound upon moving ligand into binding site] there is not only simply resistance, it is really as if it [...] I experience it as if it [ligand] moves inwardly in this position, it is as if you are on a shelf and whoop, there it [ligand] drops down [...]*
>
> Interviewer: *When you say that you 'feel' your way, what do you mean by that?*
>
> Student: *I mean that I do not base my movements on any specific theory about the exact orientations of the groups, like polar towards nonpolar or polar towards polar and so on, but rather that I try to feel my way.*

It is evident from the quote above that the student attaches his haptic experience to the intermolecular interaction between ligand and protein during interaction with the model. The student's suggestion that he "feels his way" depicts how the student exploits the force feedback to supplement his chemical reasoning with the haptic information perceived during the search process. In this way, stimulating the student to 'think aloud' offers the researcher a window into the connections between different perceptual modalities during problem solving.

In conjunction with this oral data, we also collected real-time information about students' 3D spatial interactions with the model. Specifically, the chronological sequence of students' interaction with the system was logged in the form of positions of the ligand (relative to the protein) at two-second intervals, as well as the force magnitude obtained from the potential field at each position (logged irrespective of whether students perceived haptic feedback or not). This data was used to visualize each student's movement of the ligand within a Cartesian coordinate system over time (Figure 2). Each logged position of the ligand corresponds to a sphere. Larger spheres indicate positions where the ligand experiences greater force magnitudes. Elapsed interactive time during the task is conveyed by a black-to-white shading gradient.

Figure 2 contains profiles from two students in study 1 who performed a docking task similar to the item described above. Each of the participants interacted with the model either with haptic feedback enabled (left) or disabled (right), respectively. These two patterns show marked qualitative differences. The student who docks the ligand without receiving force feedback generates a dispersed grouping of ligand positions (Figure 2, right) with no immediately observable pattern of traversal. From a purely visual point of view, the docking exploration of this student seems be rather spatially unsystematic. In contrast, consider the docking pattern revealed by a student who received haptic feedback during the task (Figure 2, left). There appears to be a more localised and channel-like quality to the visualized pattern, indicating a more 'constrained' movement of the ligand. This is further supported from numerical data retrieved from the log files. For example, it was observed that the student who produced the profile without haptic feedback (Figure 2, right), moved the ligand a total distance two-and-a-half times greater than did the student who received force feedback (Figure 2, left).

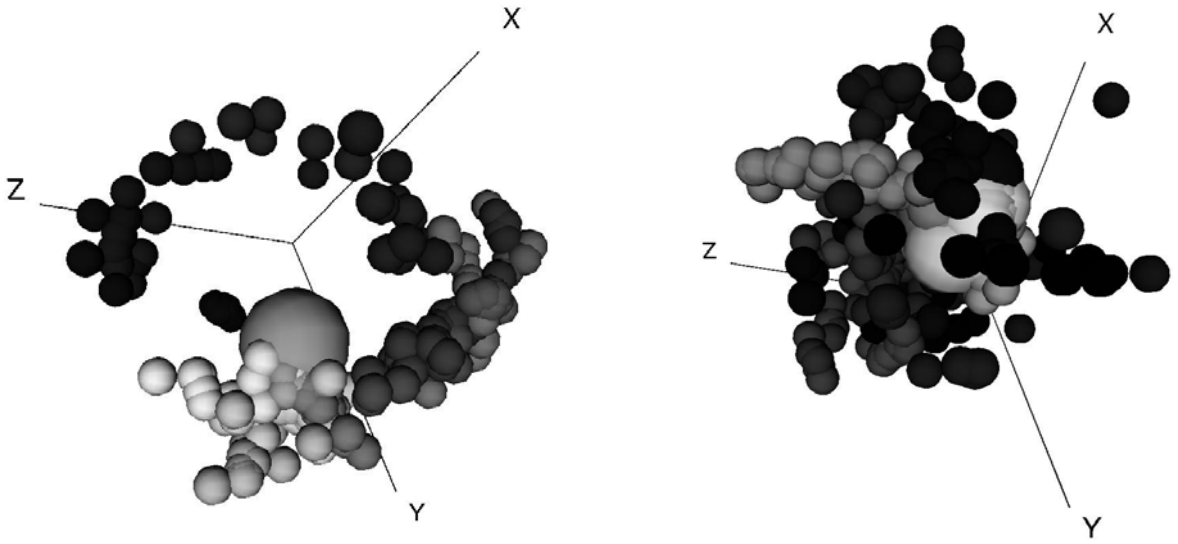

Figure 2. Examples of two students' docking profile patterns obtained with (left) and without (right) haptic feedback enabled. Shading becomes lighter as more time elapses during interaction with the model.

The methods used to visualize the patterns in Figure 2 are akin to capturing a student's docking 'journey' and externalising the resulting 'explorative sequence' adopted during a task. In conjunction with the think aloud datum presented above, the patterns in Figure 2 serve as a means of triangulation for supporting the hypothesis that force feedback induces students to 'feel out' advancement of the ligand to a feasible docking site.

Conclusions and Implications

This paper has presented methods for investigating students' learning and interaction with a haptic virtual protein-ligand docking model in response to three questions. Firstly, we measured students' learning gain through a written item in which we applied a quantitative analysis of pretest and posttest scores. Qualitative insight into the nature of individual students' learning outcomes was gained by comparing written responses before and after interaction with the model. Secondly, any changes in students' understanding were investigated by analysing the frequency of word usage in written responses. Detailed information pertaining to the construction, adjustment and replacement of students' conceptions about docking were gained through interviews. Thirdly, information about students' interactions with the model was garnered through specially designed think aloud tasks where students' were required to dock a ligand. At the same time we automatically logged 'moment-by-moment' data and visualized it to gain an appreciation of interaction patterns with the system.

Overall, in response to the need for data-gathering and analytical instruments to investigate students' learning and interaction with virtual environments in the molecular life sciences, the methods employed in our group can be used for at least three purposes, to namely:

- Obtain numerical pre/posttest scores for quantitatively measuring whether the model is associated with any learning gain.
- Characterize the nature of any learning outcomes and changes in students' biochemical knowledge by analyzing written and interview responses.
- Deliver and visualize information on students' interactive engagement with the model through think-aloud tasks and time-stamped logging data.

The methods offered in this paper have strengths and limitations. For instance, measuring learning gain informs us about the potential outcome of interaction with the system but little about the interactive process. Similarly, obtaining 'moment-by-moment' information yields a large volume of data that make analysis of students' cognitive engagement with the model a challenge (e.g. Kozma, 1991). At this stage in our research, sample sizes are small since the course is specialised and a significant amount of time is required for students to familiarise themselves with the haptic system and use it to solve tasks. Therefore, it is challenging to develop and test the presented methods with large numbers of students at varying levels as well as from different contexts. Hence, we are constantly aware of the need to reflect upon the validity (and reliability) of the instruments. Nevertheless, as evidenced in this paper, our objective has been to reconcile these caveats by pursuing a triangulated approach to data collection and analysis (e.g. Gall, Borg, & Gall, 1996). Future work will be concerned with using our results (e.g. Bivall Persson et al., 2007) to fine-tune the presented methods to explore the role of biomolecular haptic models in embodied learning (e.g. Dede, Salzman, Loftin, & Ash, 2000).

References

Bivall Persson, P., Cooper, M. D., Tibell, L. A. E., Ainsworth, S., Ynnerman, A., & Jonsson, B. -H. (2007). Designing and evaluating a haptic system for biomolecular education. *IEEE Virtual Reality Conference 2007*, 171-178. doi: 10.1109/VR.2007.352478

Dede, C., Salzman, M., Loftin, R.. B., & Ash, K. (2000). The design of immersive virtual learning environments: fostering deep understandings of complex scientific knowledge. In M. Jacobson & R.. B. Kozma (Eds.), *Innovations in science and mathematics education: Advanced designs for technologies of learning* (pp. 361-414). Mahwah, NJ: Erlbaum.

Gall, M. D., Borg, W. R.., & Gall, J. P. (1996). *Educational research: An introduction* (6th ed.). New York: Longman.

Klatzky, R.., & Lederman, S. (2002). Touch. In A. Healy & R.. Proctor (Eds.), *Experimental psychology* (pp. 147-176). New York: Wiley.

Kozma, R.B. (1991). Learning with media. *Review of Educational Research, 61,* 179-212.

Lederman, S. J., & Klatzky, R. L. (1987). Hand movements: A window into haptic object recognition. *Cognitive Psychology, 19,* 342-368.

Martin, D., Eid, M., & El Saddik, A. (2008). A haptic enabled DNA model sensing. *IEEE International Symposium on Parallel Architectures, Algorithms, and Networks (I-SPAN 2008)*, 210-215. doi: 10.1109/I-SPAN.2008.47

Minogue, J., & Jones, M. G. (2006). Haptics in education: Exploring an untapped sensory modality. *Review of Educational Research, 76,* 317-348.

Reiner, M (2004). The role of haptics in immersive telecommunication environments. *IEEE Transactions on Circuits and Systems for Video Technology, 14,* 392-401.

Srinivasan, M. A. & Basdogan, C. (1997). Haptics in virtual environments: Taxonomy, research status, and challenges. *Computers & Graphics, 21,* 393-404.

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