Scientific Applications of Force Feedback: Molecular Simulation and Microscope Control

Course notes for "Haptics: From Basic Principles to Advanced Applications," *SIGGRAPH '99.*

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Introduction

This course discusses the programming of haptic feedback devices that are part of computer graphics systems. This section of the course presents three applications and the lessons learned from them. It starts by giving a brief description of three projects at UNC that have used haptic feedback fruitfully (concentrating on two of them, the *Docker* and *nanoManipulator*). It lays out some concerns specific to implementing haptic feedback in each system and describes the solutions we found. The slides for the course presentation are included as an appendix.

Other sections of the course provide an overview of the issues involved in adding haptic feedback to computer graphics applications. For a treatment of low-level control issues, see one of several good books on robotics control, such as [Sheridan92] [Snyder85] and [Fu87]. See [Mark96] for a further discussion of the difficulties involved in such systems and the reasons for the distributed architectures found in the applications presented here.

Three UNC Applications

A growing number of applications are making good use of haptic feedback. We present here a summary of three applications developed at UNC. A more in-depth view of the first two projects (and other UNC projects not listed here) can be found in [Brooks90].

GROPE-1: An early haptic feedback application developed at UNC allowed the user to feel the effects of a 2D force field on a simulated probe, and was used to teach students in an introductory Physics course. [Batter71] These experiments were performed using a 2D sliding-carriage device that used potentiometers for position and servomotors for force presentation. Experimental results showed that haptic feedback improved the understanding of field characteristics vs. a visual-only implementation (for students who were interested in the material).

Students reported that using the haptic display dispelled previous misconceptions. They had thought that the field of a (cylindrical) diode would be greater near the plate than near the cathode, and they thought the gravitation vector in a 3-body field would always be directed at one of the bodies.

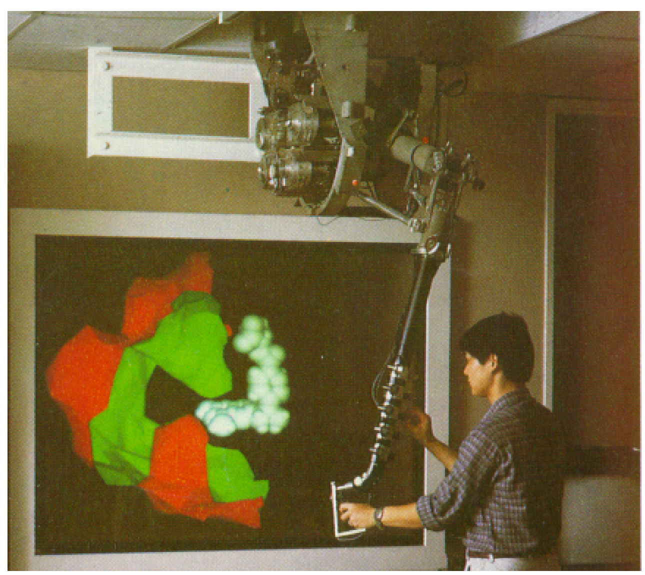


Figure 1: The *Docker* application simulates the forces between a drug and its receptor site in a protein as the user guides it to the minimum-energy configuration.

Drug Docking: Ming Ouh-young designed and built a haptic feedback system to simulate the interaction of a drug molecule with its receptor site in a protein. This system, called the *Docker*, computes the force and torque between the drug and protein due to electrostatic charges and inter-atomic collisions. These forces are presented to the user, pulling the drug towards local energy minima. This task is very similar to that of other "lock and key" applications where the user moves one object and senses collisions between it and other objects in the environment. This is a very natural application for force feedback.

The Docker system presented the force and torque vectors both visually and using haptic feedback. Experiment showed that chemists could perform the rigid-body positioning task required to determine the lowest-energy configuration of the drug up to twice as quickly with haptic feedback turned on compared to using the visual-only representations. [Ouh-young90] Scientists also reported that they felt like they had a better understanding of how the drug fit into the receptor site when they were able to feel the forces.

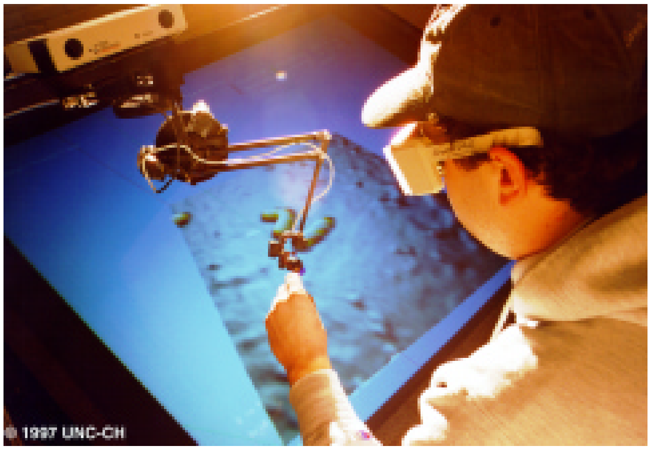


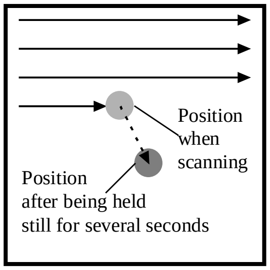
Figure 2: The *nanoManipulator* application adds a virtual-reality interface to a scanned-probe microscope. Haptic feedback allows the user to feel and modify the microscopic surface.

The Docker application, like other path-planning applications, *requires the presentation of both force and torque to the user*. Since the drug molecule is not a point probe, different portions of it can collide with the protein at the same time. Extricating the drug from a collision may require both translation and twisting. If the user is provided with only force (translation) information and no torque (twist) information, they can be led to move the drug in an improper direction.

The nanoManipulator: Figure 2 shows the *nanoManipulator* (nM) application. The nM provides an intuitive interface to scanning-probe microscopes, allowing scientists from a variety of disciplines to examine and manipulate nanometer-scale structures. [Taylor93] The nM displays a 3D rendering of the data as it arrives in real time. Using haptic feedback controls, the scientist can feel the surface representation to enhance understanding of surface properties and can modify the surface directly. Studies have shown that the nM greatly increases productivity by acting as a translator between the scientist and the instrument being controlled. [Finch95]

The haptic feedback component of our system has always been exciting to the scientists on the team; they love being able to feel the surface they are investigating. However, it is during modification that haptic feedback has proved itself most useful, allowing finer control and enabling whole new types of experiments. Haptic feedback has proved essential to finding the right spot to start a modification, finding the path along which to modify, and providing a finer touch than permitted by the standard scan-modify-scan experiment cycle. [Taylor97]

Finding the right spot



Due to time constants and hysteresis in the piezoceramic positioners used by SPMs to move the tip, the actual tip position depends on past behavior. The location of the tip for a given control signal is different if it is scanned to a certain point than if it is moved there and left constant. This makes it difficult to plan modifications accurately based only on an image made from scanned data.

Haptic feedback allows the user to locate objects and features on the surface by feel while the tip is being held still near the starting point for modification. Surface features marking a desired region can be located without relying only on visual feedback from the previous scan. This allowed a collaborator to position the tip directly over an adenovirus particle, then increase the force to cause the particle to dimple directly in the center. It also allowed the tip to be placed between two touching carbon filaments in order to tease them apart.

Finding the right path

Even given perfect positioners, the scanned image shows only the surface as it was before a modification began. There is only one tip on an SPM: it can either be scanning the surface or modifying it, but not both at the same time. Haptic feedback during modification allows one to guide changes along a desired path.

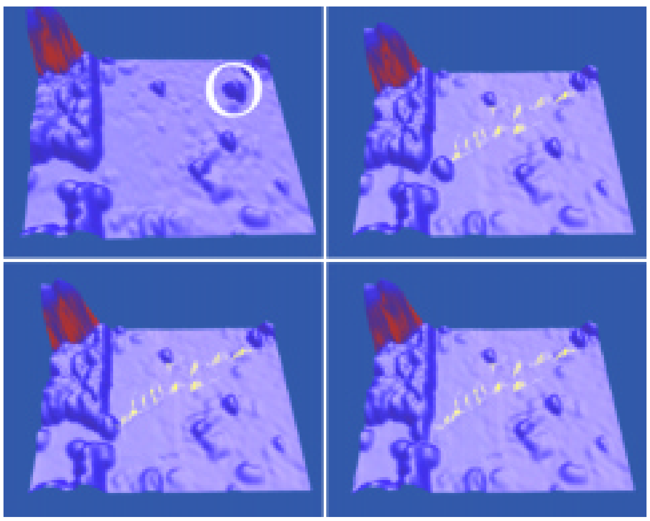


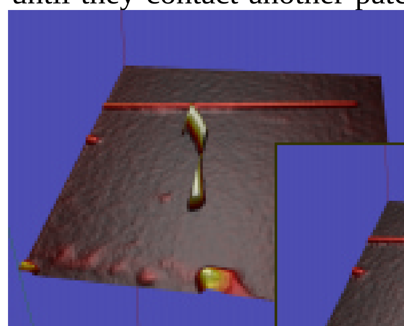
Figure 3: In this sequence of images from left to right, a 15nm gold ball (circled) is moved into a test rig. Haptic feedback is used to feel as the ball is pushed and to determine when it has slipped off the tip.

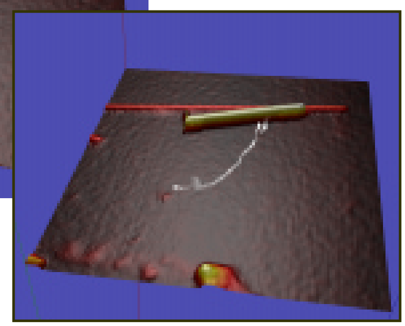
Figure 3 shows haptic feedback being used to maneuver a gold colloid particle across a mica surface into a gap that has been etched into a gold wire. This gap forms a test fixture to study the energy states of the ball. The colloid is fragile enough that it would be destroyed by getting the tip on top of it with modification force or by many pushes. This prevents attempts to move it by repeated programmed “kicks”. Haptic feedback allowed the user to tune the modification parameters so that the tip barely rode up the side of the ball while pushing it. This allowed the guidance of the ball during pushing so only about a dozen pushes were required.

Haptic feedback was also used to form a thin ring in a gold film. A circle was scraped to form the inside of the ring, leaving two “snow plow” ridges to either side. By feeling when the tip bumped up against the outside of the outer ridge, another slightly larger circle was formed. This formed a thin gold ring on the surface.

A light touch: observation modifies the system

When deposited on the surface, carbon nanotubes are held in place by residue from the solution in which they are dispersed. On some surfaces, the tubes slide freely once detached from the residue until they contact another patch of residue or another tube. Even the light touch of scanning causes them to move. By using only touch mode and switching between imaging and modification force, we have been able to move and re-orient one carbon tube across a surface and into position alongside another tube. Once settled against the other tube, it was stable again and we could resume scanning to image the surface. Haptic feedback and slow, precise hand motion (“haptic imaging”) allowed us to find the tube at intermediate points when we could not scan. The fact that the surface cannot be imaged at intermediate stages prevents this type of experiment from being performed using the standard scan-modify-scan cycle.





Haptic feedback requirements of the nM

The nanoManipulator application only requires the presentation of forces to the user (not torques), since it is displaying the results of pushing on a surface with a point probe. This allows the use of a haptic feedback device that only produces force output. It is helpful to have both position and orientation as input, since the same

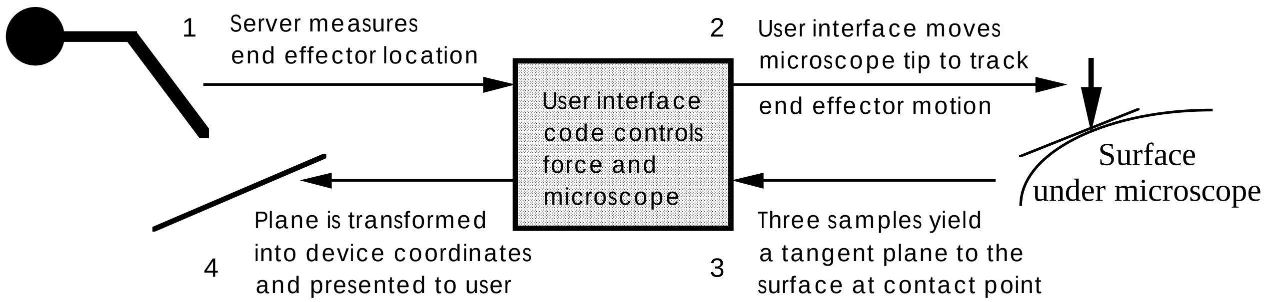


Figure 4: The nanoManipulator application determines a local plane approximation to send to the force server. As the end effector moves, the microscope tip tracks it on the surface and sends a new plane equation describing the local surface.

haptic device can be used to position and orient the surface for viewing.

The graphics part of the nM only requires a frame update rate near 20 Hz while the stable haptic presentation of hard surfaces requires an update rate of more than 500 Hz. Thus, it is clear that *the force-update loop must not be limited to the speed of the rest of the application*. In fact, since the force loop must be guaranteed to maintain its update rate at the risk of instability, it was necessary to dedicate a separate process to drive the force display. Thus, the application is split into two or more separate processes.

Figure 4 shows one solution, which splits the application between three computers that communicate over a network. One computer controls the microscope, one controls the haptic device and one controls the user interface and graphics. The haptic controller maintains a 1kHz update rate between the user's hand and a local plane approximation to the surface. The application updates this local approximation 20 times per second. Similarly, the microscope controller maintains constant tip-to-surface contact and receives requests to sample new locations at the rate of 20 times per second. A more complete description of this operation is found in [Mark96].

Conclusion

The three applications presented here indicate that force feedback can be a useful addition to a computer graphics application. They all share the need to display some sort of force field to the user, whether simulated or a representation of a remote but physical surface.

We have found that haptic feedback gives improved situational awareness in the applications we have built. It can give students a better understanding of force fields and build a scientist's intuition about a problem. Force feedback is especially good for manipulation tasks, where the user is moving a real or simulated object as part of the task.

Further Information

More information on haptic feedback at UNC is at http://www.cs.unc.edu/Research/force/. Information about the Docker project can be found at http://www.cs.unc.edu/Research/graphics/GRIP/. Information about the nanoManipulator can be found at http://www.cs.unc.edu/Research/nano/.

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