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Project GROPE – Haptic Displays for Scientific Visualization

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ABSTRACT

We began in 1967 a project to develop a haptic+ display for 6-D force fields of interacting protein molecules. We approached it in four stages: a 2-D system, a 3-D system tested with a simple task, a 6-D system tested with a simple task, and a full 6-D molecular docking system, our initial goal. This paper summarizes the entire project—the four systems, the evaluation experiments, the results, and our observations. The molecular docking system results are new.

Our principal conclusions are:

- Haptic display as an augmentation to visual display can improve perception and understanding both of force fields and of world models populated with impenetrable objects.
- Whereas man-machine systems can outperform computer-only systems by orders of magnitude on some problems, haptic-augmented interactive systems seem to give about a two-fold performance improvement over purely graphical interactive systems. Better technology may give somewhat more, but a ten-fold improvement does not seem to be in the cards.
- Chemists using GROPE-III can readily reproduce the true docking positions for drugs whose docking is known (but not to them) and can find very good docks for drugs whose true docks are unknown. The present tool promises to yield new chemistry research results: it is being actively used by research chemists.
- The most valuable result from using GROPE-III for drug docking is probably the radically improved situation awareness that serious users report. Chemists say they have a new understanding of the details of the receptor site and its force fields, and of why a particular drug docks well or poorly.
- We see various scientific/education applications for haptic displays but believe entertainment, not scientific visualization, will drive and pace the technology.
- The hardware-software system technology we have used is barely adequate, and our experience sets priorities for future development.
- Some unexpected perceptual phenomena were observed. All of these worked for us, not against us.

KEYWORDS: haptic, force, tactile, scientific visualization, interactive graphics, virtual worlds.

CR CATEGORIES: I.3.6 Computer graphics interactive techniques. J.3 Biology.

1. INTRODUCTION

1.1 Scientific Visualization

Scientific visualization aims to help scientists make discoveries by improving their perception of data describing the natural world and of predictions of computer models of the natural world [15]. Scien-

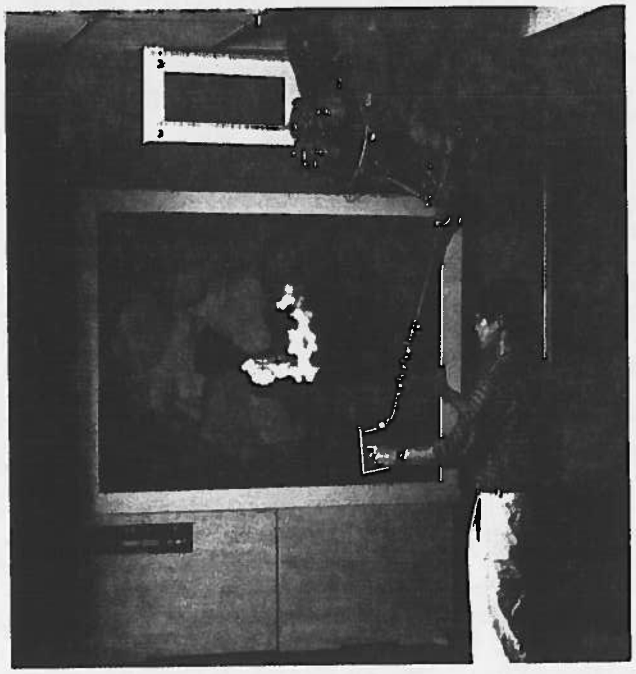

Figure 1. GROPE-III haptic display system in use.

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[†] Deceased. Mr. Batter died before completing his Ph.D. dissertation. This paper includes his description, results, and observations on the GROPE-I system and experiments.

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+Haptics—"pertaining to sensations such as touch, temperature, pressure, etc. mediated by skin, muscle, tendon, or joint." [29].

any perception augmentation?

A4. The technologies (servo control systems, etc.) we are using are marginally adequate. Indeed, they may be limiting the performance enhancement we observe. (Or they may not. We may be seeing all the performance gain there is to see.)

We find update rate to be critical. We get a marginally useful system at 20 updates/second; good performance on hard-surface forces requires 60-80 ups with our mechanisms.

System lag is crucial. Ours works with lag less than or equal to one update/frame. We have not measured when lag cripples a high-update-rate system [23].

Force and torque resolution and accuracy do not seem to matter much, because of the closed-loop perception-manipulation system of the user. Quantization error on input does matter.

Mechanical backlash, static friction, and other discontinuities are very troublesome. Ordinary dynamic friction is not a major problem. Indeed, one has to have enough to critically damp the servo systems.

We have used finger-hand manipulation in a 2"x 2" working area and hand-arm manipulation in a 3'x 3'x 3' working volume. We believe finger-hand manipulation in a 4" x 4" x 4" working volume would be better than either. One may have to move elbow and shoulder, with or without force diplay there, to allow full manipulation and force-torque sensing with fingers and wrist.

Q5. What is the perception yield curve for haptic technology enhancement? Where does it approach saturation?

A5. With our mechanism, 80 ups should suffice. However, we measure continuing performance improvement in a texture-perceiving task as update rate is advanced from 500 ups to 1000 ups, which we partly understand.

4. THE HAPTIC SYSTEMS AND EXPERIMENTS

4.1 GROPE-I: Haptic Display Improves Perception of Continuous 2-D Force Fields—*Batter* [1]

Task: Examine simple force fields by moving a probe particle, seeing and feeling the force on the probe. Then, for test fields, draw the force vector length and magnitude, given a probe position and no time to calculate.

Apparatus: A small knob attached to a movable platform that can be positioned within a horizontal plane two inches square. Potentiometers sense its x and y positions; servomotors exert x and y forces (Figure 2). Both are connected to the computer driving an associated visual display.

As the user moves the knob on the force display device, a visual cursor follows his motion. At the same time, he experiences a force. The magnitude and direction of this force is also indicated on the screen by a vector originating at the position of the probe. The force and visual displays are recalculated at approximately 12 ups.

Subjects: Thirty-four freshman physics students who had not studied force fields. The participants were paid according to their performance.

Procedure: The subjects, randomly divided into test and control groups, were given six hours of lecture on force fields and a pretest examination.

Each student was asked to "map" five fields, given a diagram with the center of the field indicated. The students were asked to estimate the magnitude and direction of the force by drawing vectors at ten given probe positions.

After the pretest, each student examined some 16 force fields in two hours of exercises. The members of the test group received force feedback while members of the control group did not. This was accomplished by unplugging the servo motors for the control group. This ensured that all visual displays, timings, etc., were identical for the two groups. When all the students had completed the exercises, another examination like the pretest was given.

Results: The experiment was repeated three times. The subjects for Group A were science majors from an honors section. This group's learning was better than the control group's, a difference significant at the 2.5% level.

Subjects for Group B were students from a physics section for non-science-majors. The results for Group B were quite different. Only slight improvements were noticed, explainable by chance. Puzzled, we selected a third group, once again from a science-major section. The Group C results replicated those of Group A.

The qualitative observations offered a clue. The science-oriented students showed greater interest in the material presented and in using the device. The non-science students tended to watch the clock. The science students became deeply involved in the use of the device, whether force feedback was present or not. They seemed oblivious to other activities in the room, and their attention could be attracted only with difficulty. Many of these students talked to themselves (as did subjects in later experiments).

An update rate of 12 ups was satisfactory for these continuous force fields.

Comments: A tool can be useful only when the user wants to use it. Our monetary incentives were insufficient to motivate Group B. Groups A and C, the honors sections, found interest and inherent motivation in the experiment, with or without force feedback.

We were surprised and puzzled by this result. We had expected the display and manipulation to add enjoyment and motivation, closing the gap between those of low and high intrinsic motivation. Instead, to those who had much, more was given by the more powerful tool. Those who had little were less helped.

Students reported that using the haptic display dispelled previous misconceptions. They had thought 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

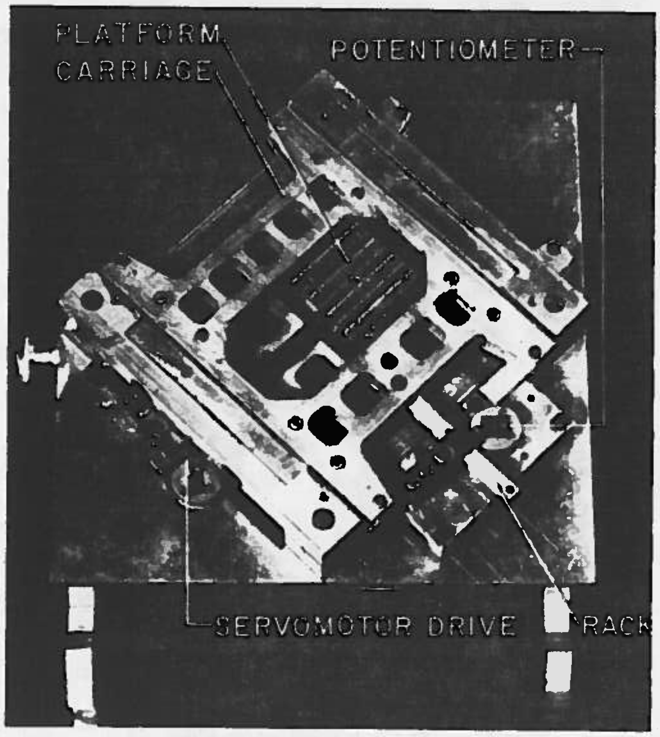

Figure 2. The GROPE-I device.

a hypothesis about its structure which he uses to predict how it will look from other viewpoints. He believes one tends to select the most probable structure to hypothesize, making it "difficult, perhaps sometimes impossible, to see very unusual objects."

We postulate, based on Kilpatrick's observations and Batter's, that displayed forces are similarly interpreted as the most likely forces. Since we commonly experience only constant or linear force fields, these are the only ones we interpret correctly. Batter found, for example, that subjects were unable to distinguish among square-law and cube-law fields without direct comparison.

4.3 GROPE-IIIA: Haptic Display Alone Can Be Better Than Visual Display Alone for Simple Force Fields—*Ouh-Young* [19]

Task: Find the minimum-energy position and orientation of a virtual bar suspended in space by six springs with random anchor points and elastic constants (Figure 5).

Apparatus: The Argonne ARM is attached to a dedicated Sun4. Visual display is on an E & S PS-330 color vector display. Stereo vision is provided by a Tektronix alternating polarization plate and polarized glasses. The user can use the handgrip to change viewpoint location and viewing orientation, and to manipulate the bar.

The user has an auxiliary control, held in the free hand, which gives viewpoint rotation about the Y-axis of the virtual world, to give kinetic depth effect. The use of this aid costs time; subjects used it less than 20% of the time.

On the screen there are two colored spheres landmarking the virtual space. They are unrelated to the docking task, but provide visual cues to the relative positions of objects in the virtual world. The springs are invisible (Figure 6).

A New Visual Representation of Forces and Torques: The resultant of all translational forces on an object is represented as a 3-D vector with one end fixed at the center of a sphere located at the geometric center of the object. The resultant of all torques on an object is represented as a pair of 3-D vectors tangent to the sphere. Vector lengths are proportional to the forces and torques. Visually these vectors would appear as three springs attached to the sphere—one pulling the sphere through the center, the others, tangent, rotating the sphere.

There are infinitely many equivalent torque vectors tangent to a sphere. For any non-zero torque, there are exactly two with origins on the occluding contour of the sphere (except for the degenerate case where all torque vectors are parallel to the viewing plane). We display only the one of these that is not itself occluded by the sphere. Figure 6 shows this visual representation.

Subjects: Seven volunteer computer science students and staff. All subjects were able to see stereo. One subject (S2) was very experienced in using the ARM; the others were relatively inexperienced.

Procedure: We studied performance with only force feedback (F) and with only visual presentation of force and torque vectors (V).

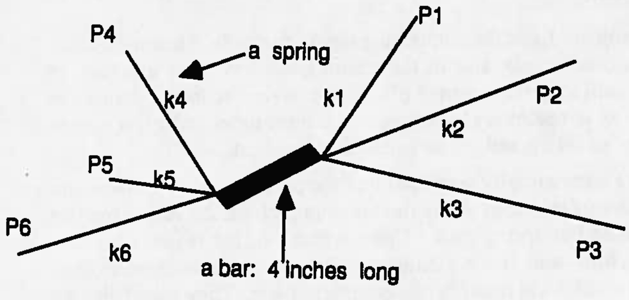

Figure 5. The simplified docking task. The goal is to find the zero-force position and orientation of the bar, where P1 to P6 are positions in 3-D, and k1 to k6 are the elastic constants for springs.

Our hypothesis was that F would have a significantly lower potential energy level after 15, 30, 45, and 60 seconds in a 60 second trial.

For each trial, the subjects were told to reduce the system energy by minimizing the forces and torques. They were told to do the tests as fast as they could in 60 seconds. Each subject participated in two sessions: an hour of training one day; and an hour of experiment the next day. Each subject was trained until performance stopped improving. Training generally took about 20 minutes for F but about 40 minutes for V.

Design. Each of the six trials used gave the subject an initial random configuration of the springs. The within-subject design is a one-way analysis of variance with a Latin square of repeated measures. The same six trials were used for each method by each subject, but the trials were disguised by changing the initial viewpoint each time.

Results. Figure 7 shows completion times and the potential energy after 60 seconds. Energy levels were significantly lower with F than with V at 15, 30, 45, and 60 seconds. We observed that most subjects using F had reached steady state by 30 seconds into a trial. Some subjects reached steady state using V after 30 seconds, but many were still improving their docking position at 60 seconds.

Comparing the mean completion times for the two methods shows a haptic performance advantage of 2.2 times. Almost all subjects reported surprise that they could do blind docking at all, much less that they could do it faster than visual docking. This result may be true only for energy spaces with only one minimum.

The mean final energy for F was half as large as that of V, i.e., F users got better docking when they ran for the same time.

Comments:

- Since this energy space has only one minimum, this is really a toy problem better solved by computation than by interaction. Indeed, if the force-driven arm is just turned loose, it makes its way to the global minimum. Hence results from this experiment should not be generalized.

- Our visual presentation of the forces and torques are two independent vectors. During the visual docking, we observed that the subjects dealt with force and torque vectors separately. Most subjects shorten the force vector first and then the torque vector. This is not always the best way of minimizing energy. When the subjects were docking using force, they did translation and rotation at the same time in continuous motion. F's being twice as fast as V also suggests that subjects treated forces and torques as independent entities when working visually.

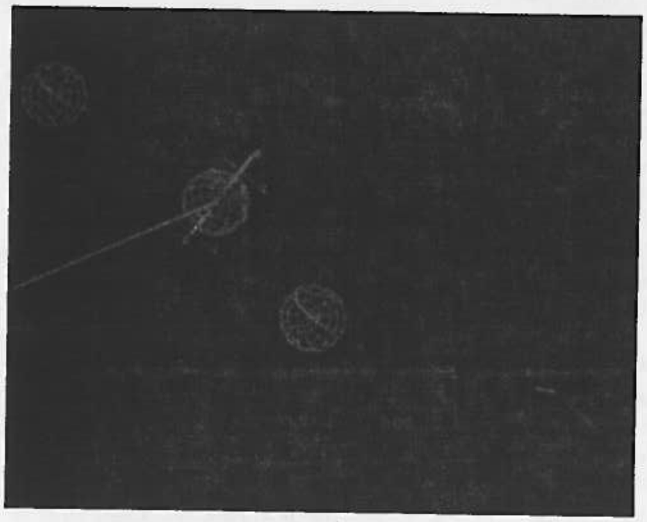

Figure 6. Visual display for GROPE-IIIA.

creases inter-subject variance. Nevertheless, the molecular docking results describe the real-world effect more realistically than do the bar-spring results.

- A performance experiment of this kind was the best we could devise to get a quantitative evaluation of the power of haptic visualization. The greatest promise of the technique, however, lies not in time saving but in improved situation awareness. Chemists report getting better comprehension of the force fields in the active site and of exactly why each particular candidate drug docks well or poorly. From this improved grasp of the problem, one hopes users would get whole new hypotheses and ideas for new candidate drugs. This we cannot measure, and we do not yet have any anecdotal evidence. Research chemists are now investing their professional time in using this system on their problems.

5. HARD-SURFACE FORCES, SYSTEM STABILITY, AND MECHANICAL IMPEDANCE STUDIES

5.1 Hard-Surface Forces Are Hard—*Kilpatrick* [13]

No two atoms can occupy the same space at the same time—the repulsive force rises as r to the -13, where r is the inter-atomic distance! Modeling such hard-surface forces is difficult with most haptic displays. It is essentially the same as demanding a square-wave response from a second-order servo system. Two problems arise. First, even in a linear analog system, there is no force applied until the probe has overshot, penetrated the virtual surface. The system has inertia and velocity. Unless it is critically damped, there will be an unstable chatter instead of a solid virtual barrier. Second, digital systems do quantized time-sampling. Quantization effects, sampling effects, and computational lags add new causes for instability.

One solution is to provide a brake—a variable damping system that radically increases friction when a virtual hard surface is encountered [22]. This requires measuring the force the user is applying to the damped system, and removing braking when he attempts to move away from the surface.

In the GROPE-I system we modeled only continuous forces (up to r to the -3 power), so did not encounter the problem. In GROPE-II, we adjusted system damping to keep stability, and approximated hard surfaces as Hooke's Law elastic surfaces with adjustable elasticity. Even though the virtual blocks, table, and tongs were in fact rather mushy, with millimeter-scale deformations, they did not *feel* that bad.

Kilpatrick augmented the haptic display with clicks whenever virtual contacts were made. This helped the haptic illusion noticeably.

5.2 System Stability and Responsiveness—*Ouh-Young* [20]

Following Hogan [12], Ouh-Young has published a true discrete analysis of the system composed of the Argonne ARM and the human arm driving it.

Parameters were measured by using a 2-D high-performance haptic display system built by Minsky and Steele [16]. This system is capable of very fast sampling and force response, up to 1000 ups.

The analysis and measurement show that 80 ups should give as good behavior to our ARM-arm system as the human can perceive. Lighter-scale, finger manipulation systems would require higher update rates.

A puzzle arising in these measurements is that users can in some cases perceive incremental simulation quality when the joystick update rate is increased from 500 ups to 1000 ups, even though the muscle-nerve system is theoretically incapable of sensing such frequencies. Our explanation is that although the joystick is running at 500 Hz, it may be unstable at that frequency when it is stable at 1000 Hz. The vibrations caused by this instability can be sensed by the human hand. When the system is stable at both sampling rates (500 Hz and 1000 Hz), we observe that there are no gross differences in force perception in a few simulations in Minsky's Sandpaper environment.

6. OBSERVATIONS

6.1 Indirect Force Perception

The molecular docking task not only requires the small drug molecule to be positioned in translation and rotation, but also requires the user to change the conformation of the drug molecule to get best fit into the active site. This is done by manipulating up to twelve twistable bonds in the drug, each represented by a 1-D dial mounted on the ARM shaft (Figure 1). Docking is thus seeking an energy minimum in an 18-D space. (In our controlled experiments, all bonds but six were preset to optimum values, and users had to seek optima for only six bond twists, or 12-D in all.)

Typical user action is to do bond twists, one at a time, with the left hand, then adjust 6-D position with the handgrip in the right hand.

The ARM delivers forces only in the six positioning dimensions; we have not yet mounted force motors on the bond-twist dials. Nevertheless, we observe that one perceives force feedback as he twists a bond dial. The forces on the right hand change as the left hand manipulates a dial; the brain integrates the two into an action-reaction perception.

6.2 Display to Fingers-Hand versus Display to Hand-Arm

The GROPE-I experiments used a finger-grip display. Most joint action was at the wrist and outward. The GROPE-II and GROPE-III experiments used a hand-grip display with joint action at the shoulder and outward. We used the Argonne ARM because it was built and available to us; a 6-D finger-movement force-torque display was and is not available, although several research groups are now engineering such.

Based on our experience we would prefer to do our future work on a finger-hand display because:

- It is less tiring to use, since the elbow can be separately supported. To our surprise, however, none of our users complained of fatigue in the GROPE-III experiments, in spite of sessions lasting 2.5 hours. Most chose to stand, rather than using a stool.
- The relative manipulation resolution of the finger-hand muscles is at least as good as that of the hand-arm system [17]. Absolute resolution does not matter.
- The relative force-perception resolution of the finger-hand system seems at least as good as that of the hand-arm system.
- It is simpler and more economical to have hand-scale working volumes reflected in similar-scale visual displays than arm-scale ones. For GROPE-IIIB exploratory experiments we used a rear-projection screen to give comparable visual and haptic working volumes. For GROPE-IIIB formal experiments we used a visual working volume much smaller than that of the manipulator. The scale discrepancy did not bother any of our users—people instinctively normalize it out.
- Cost should be lower because everything is smaller, including motors and power requirements.

6.3 Better Visual Interactive Docking As a By-Product

Pursuing effective interactive docking with the GROPE-III System led Ouh-Young to a new visual docking technique that can be implemented on any workstation, without a haptic display.

Ouh-Young discovered that the force-torque display of Figure 6,

in a peg-in-hole manipulation task with force feedback. Paper presented at Thirteenth Annual Conference on Manual Control, MIT (June 15-17, 1977).

[11] Hill, J.W. and Salisbury, J.K., Jr. Study to design and develop remote manipulator system. *Quarterly Reports 5*, 6 (January 1978). Stanford Research Institute, Menlo Park, CA.

[12] Hogan, N. Stable execution of contact tasks using impedance control. *Proceedings of IEEE Robotics and Automation Conference*, Raleigh, NC (1987), 1047-1054.

[13] Kilpatrick, P.J. *The Use of Kinesthetic Supplement in an Interactive System*. Ph.D dissertation, Computer Science Department, University of North Carolina at Chapel Hill, 1976.

[14] Kuyper, L. Receptor-based design of Dihydrofolate Reductase inhibitors: Comparison of crystallographically determined enzyme binding with enzyme affinity in a series of carboxy-substituted Trimethoprim analogues." *J. Med. Chem.. 1122*, 25 (1982), 1120-1124.

[15] McCormick, B.H. , DeFanti, T.A., Brown, M.D., eds. Visualization in scientific computing. *Computer Graphics 21*, 6 (Nov. 1987), and *SIGGRAPH Video Review*, Issues 28-29 (Nov. 1987).

[16] Minsky, M., Ouh-young, M., Steele, O., Brooks, F. P., Jr., Behensky, M. Feeling and seeing: Issues in force display. *Proc. of 1990 Symposium on Interactive 3D Graphics*, Snowbird, Utah, March 1990. Published in *Computer Graphics 24*, 2 (March 1990), 235-244.

[17] Mowbray, G. H. and Gebhard, J. W. Man's senses as information channels. In H.W. Sinaiko, ed. *Selected Papers on Human Factors in the Design and Use of Control Systems*. Dover: New York, 1961. p. 118.

[18] Ouh-Young, M., Pique, M., Hughes, J., Srinivasan, N., Brooks, F.P., Jr. Using a manipulator for force display in molecular docking. *Proc. IEEE Robotics and Automation Conference 3* (Philadelphia, April 1988), 1824-1829.

[19] Ouh-Young, M., Beard, D.V., Brooks, F.P., Jr. Force display performs better than visual display in a simple 6-D docking task. *Proc. IEEE International Conference on Robotics and Automation* (Arizona, May 1989), 1462-1466.

[20] Ouh-Young, M. *Force Display in Molecular Docking*. Ph.D. Dissertation, Computer Science Department, University of North Carolina, Chapel Hill, 1990.

[21] Pattabiraman, N. et al. Computer graphics and drug design: Real time docking, energy calculation and minimization. *Journal of Computational Chemistry 6* (1985), 432-436.

[22] Smith, M.J. *Tactile Interface for Three-Dimensional Computer-Simulated Environments: Experimentation and the Design of a Brake-Motor Device*. M.S. Thesis, Mechanical Engineering Department., Massachusetts Institute of Technology, 1988.

[23] Stark, L.W. , Kim, W.S., Tendick, F. Cooperative control in telerobotics. *Proc. IEEE International Conference on Robotics and Automation* (Philadelphia, April 1988), 593-595.

[24] Steelman, H.S. *The GROPE-1 System: An Analysis of Friction and Backlash Problems*. M.S. Thesis, Computer Science Department, University of North Carolina, Chapel Hill, 1968.

[25] Sutherland, I.E. The ultimate display. *Information Processing 1965*, *Proc. IFIP Congress 65*, 506-508.

[26] Turk, G. *Interactive Collision Detection for Molecular Graphics*. M.S. thesis, Computer Science Department, University of North Carolina at Chapel Hill, 1989.

[27] Weber, C.O. The properties of space and time in kinaesthetic fields of force. *Am. J. of Psychology 38*, 4 (1927), 597-606.

[28] Weber, C.O. The properties of space and time in kinaesthetic fields of force. *Am. J. of Psychology 41*, 1 (1929), 95-105.

[29] *Webster's New International Dictionary*. 2nd ed. Merriam: Springfield, MA.