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VIRTUAL REALITY AT WORK

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1. INTRODUCTION

The utility of virtual reality computer graphics in telepresence applications is not hard to grasp and promises to be great. When the virtual world is entirely synthetic, as opposed to real but remote, the utlility is harder to establish. Vehicle simulators for aircraft, vessels, and motor vehicles are proving their worth every day. Entertainment applications such as Disneyworld's StarTours are technologically elegant, good fun, and economically viable. Nevertheless, some of us have no real desire to spend our lifework serving the entertainment craze of our sick culture; we want to see this exciting technology put to work in medicine and science.

2. TESTING A FORCE DISPLAY FOR SCIENTIFIC VISUALIZATION: MOLECULAR DOCKING (Ming Ouh-Young)

2.1 The technology. This test uses a Model E-3 Argonne Remote Manipulator (the ARM) that offers a full 6-D input position sensing and full 6-D force and torque output. A Sun 4 provides computational power and ARM control; and E.&S. PS-300 provides the visual output. A Tektronix stereo plate is used with passive circular polarizing glasses.

2.2 The molecular docking application. The enzyme dihydrofolate reductase binds to a variety of inhibitors, natural and synthetic. Of twelve inhibitors studied by our collaborators at Burroughs-Wellcome, the precise structure of the enzyme-inhibitor complex is known for six.

Binding energy is a complex function of atomic positions, involving Coulomb forces, van der Waals forces, nuclear forces, hydrogen-bonding forces, and thermodynamic forces. With 6 degrees of freedom in the drug docking, and up to 12 twistable bonds in the drugs, the docker is attempting to find a global minimum of the energy in a space of up to 18 dimensions, a space pock-marked with local minima. Brute-force algorithmic methods would require years of computer time to explore the space.

It is hard to imagine a visual display that would effectively produce all the needed insight to enable a user to manually dock the drug so as to minimize energy. We postulated that *feeling* the forces, particularly the (1/r)**7 and (1/r)**13 forces that define the receptor pocket, would substantially help chemists in manual docking.

2.3 The experimental results. Chemists can dock an inhibitor in about 25 minutes using our force display system. Ming's controlled experiments indicate an upper bound of about a factor of two improvement in docking performance when the visual display is aided with our force display. Our force display has many primitive characteristics, so there is hope for some improvement in this number, but an order-of-magnitude improvement doesn't seem to be in the cards.

2.4 Whither now? We plan to get some actual drug-design experience with real drug designers. We also want to build or buy a finger-scale, versus arm-scale, 6-D force output device. The literature suggests that resolution should be at least as good with the scaled-down device, and stability and ease of use much better.

3. TESTING A HEAD-MOUNTED DISPLAY FOR SCIENTIFIC AND MEDICAL VISUALIZATION (James Chung)

3.1 The technology. We use the standard available technology: tiny TVs and Polhemus trackers. Our PixelPlanes graphics engine is faster than almost all of today's delivered engines. The Polhemus has respectable frame-rate but unacceptable lag for head-mounted displays. We measure 250-400 msec., and lag seems to depend upon source-sensor distance. We are pursuing several new tracker technologies.

3.2 The only advantage of head-mounted displays - intuitive navigation. Considered cold-bloodedly, today's head-mounted displays have many disadvantages: resolution, sharpness, field-of-view. Their inherent comparative advantage is intuitive navigation of the virtual space. It should be much easier for the user to know where he is and what he is looking at than in through-the-window graphics. How much is this worth? How much does it improve performance in a real application?

3.3 The radiation-treatment planning application. Radiation oncologists have to plan the shape, intensity, and direction of multiple beams of radiation so as to burn the tumor without burning other sensitive or vital organs. This task requires imaginative use of 3-space, a good image of the anatomy of the patient, and, ideally, real-time calculation of the dose to the tumor and to unwanted organs.

3.4 The planned tests. We have volume-visualized MRI anatomical data on tumor patients. Our collaborating radiologists, in a controlled experiment, will devise treatment plans using the head-mounted display versus through-the-window graphics. We will measure task time and goodness of plan as experimental variables.