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Technical Note

1971-38

Kineticonics and Molecules

R. N. Davis
J. J. FitzGerald

16 September 1971

Prepared under Electronic Systems Division Contract F19628-70-C-0230 by

Lincoln Laboratory

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Lexington, Massachusetts



A1D0731546

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MASSACHUSETTS INSTITUTE OF TECHNOLOGY
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R. N. DAVIS
J. J. FITZGERALD

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The work reported in this document was performed at Lincoln Laboratory, a center for research operated by Massachusetts Institute of Technology, with the support of the Department of the Air Force under Contract F19628-70-C-0230.

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ABSTRACT

Evolution of the ability to compute molecular models inevitably leads to exploration of the ways in which models may be converted from computed bits and bytes into readily perceivable mental imagery.

Computer-generated dynamic graphic methods may be used to provide enhanced understanding for research, technical reporting, technical explanations, and education.

Accepted for the Air Force
Joseph R. Waterman, Lt. Col., USAF
Chief, Lincoln Laboratory Project Office

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KINETICONICS AND MOLECULES

I. INTRODUCTION

Motion is a very powerful phenomenon for producing mental imagery and understanding of time-dependent relations. Motion may also be used to provide understanding of spatially related physical objects and to assist in the perception of nonphysical concepts and phenomena.

Computer animation is now generally considered to be the production of motion pictures resulting from computing and is a subset of dynamic graphics. Film is a convenient, long-term storage medium. The important aspect is the human brain producing meaningful mental imagery from the computer bits and bytes, irrespective of the specific mechanisms used in the process.

I use the word "Kineticonics," meaning energetic motion imagery, to convey the ideas of energetic impact upon the perceiver, to imply understandable mental imagery, and to avoid the confusions related to the specific channels from the computer to the brain.

For the sake of brevity, I shall assume your understanding that a series of related still images presented to the retinas of the eyes in an appropriate time sequence will produce motion imagery, and that there are ways in which computing techniques may cause these presentations whether they are via oscilloscopes, film, or some other media.

Research psychologists may define as many as a thousand separate visualizing "cues." You will not want, nor will you need, to consider more than a few of these to be able to produce quite satisfactory computed Kineticonics.

We shall not concern ourselves at this time with the various possible "models" of the brain, but shall recognize that it is a very complex mechanism and accomplishes many wonderful perceptions. In fact, the brain is so profound that it will assemble a perception (or perceptions) from almost any set of inputs.

II. BALL AND STICK MODEL

If I hand you a ball-and-stick model of a complex molecule, you grasp it; you may then tip or rotate it as you examine it. What visual cues are you using for building your mental perception? Rotation is one, to provide various viewpoints. You move it sideways, or up and down. Translation provides viewpoints. You may move it away, or closer. Magnification or zooming lets you perceive various degrees of detail. As you perform these motions, you are "windowing," "clipping," or "scissoring" so that you can pay attention to various degrees of complexity. You are seeing the forest, sorting out the trees from the forest, the leaves from the trees, the mites, the ticks, and the mosses. Your perspective and depth perception are working for you. You may be looking through the front portions to examine more closely the interior detail. Your brain uses "convergence" and "accommodation" relations to help delineate; "hidden" lines and surfaces become apparent. The balls and the sticks may be colored. These colors aid in building your mental perception, and are important when you analyze or describe the observations you are making.

Notice that the motions you have been using are solely to gain advantageous viewpoints, not to examine time-dependent relations.

If I give you another small ball-and-stick model, you may try to attach it to the previous model, using your ingenuity and within the rules established for building molecules. Using the rules, you may build ever greater models while exploring existing rules and phenomena.

As you build your great molecule or crystal model, you might decide to photograph it. Now you are concerned with light, light direction, shadows, possibly even textures, as well as the camera's viewpoint. You may wish to make a movie of the various stages of the development. If so, then you add sound, voice for explanation, characteristic sounds for effect, and music for interest and emphasis. You also might like some art. Life has become complicated!

Appropriate computing environments can provide suitable ways of including all the foregoing "visualizing cues" and many more. Rules may become computing algorithms.

III. STUCK WITH STICKS?

The magnificent book, "The Architecture of Molecules," by Pauling and Hayward¹ demonstrates that the sticks of our model are convenient physical necessities, they provide a symbology for understanding, and are poor representations of the elastic forces and the resultant motion. Would the balls be better represented as fuzzy vibrating volumes? Few people would dare to compete with Roger Hayward in his artistry and understanding, but not even Roger would undertake to hand-animate a movie demonstrating the various vibrational modes of the ammonia molecule. Dynamic computer graphics can be used to provide mental imagery that otherwise cannot be achieved. Combinations of real life, high speed, time lapse, special effects, and computer animation photography have demonstrated the value of Kineticonics for enhancing understanding.²

IV. THERAPEUTIC MATHEMATICS

Rotational therapy for Kineticonics may not be mathematically complicated, can lead to simple computing equations, and can be one-, two-, or three-axis rotation. Translation and magnification are simple. The equations for perspective and "two-eye" depth perception or stereo may be derived from normal geometric projection concepts. However, if you manipulate your scene so that parts of it pass beyond the presentation "window" of your system, you may destroy your presentation. There are hardware and software cures and safeguards for windowing and scissoring. Ivan Sutherland³ provides more information in his article "Computer Displays" in a recent Scientific American.

The representation of surfaces may be simple or not, depending on the surface and your desired treatment. Planes and surfaces of revolution tend toward the simple, while warped and exotic ones may approach the very difficult. We have found that non-patterned, or "random," dots can be easily used for delineating many kinds of surfaces. They have also been extensively used in psychological and stereology studies.

Treatment of hidden lines and surfaces has received a great deal of excellent attention, but is still a challenging problem. Some reasonably simple

special-purpose solutions are available, but the current general-purpose approaches tend to require great amounts of computing time. Sometimes, stereoscopy can be helpful in avoiding the necessity of removing the hidden parts because the perceiver can focus his attention in depth, delineating that which he wishes to examine.

V. INTERACTIVITY

The advent of time sharing with interactive keyboards and local typing are obvious demonstrated virtues. The addition of a local display permits much more rapid construction and correction of one's "thinking." Continuous concentration on the subject is important. Writing tablets, light guns, "bugs," "rotatable knobs," and "joy sticks" provide much enhanced capability. We see storage tube displays exploding into the static graphic endeavors, dynamic displays appearing in some environments, and computing languages becoming more user-oriented. The aim of all these endeavors should be to reduce the attention a user must pay to manipulations so that his total mental exercise can be directed toward the subject.

VI. THE CINE QUALITY SPECTRUM

Let us now consider several grades of computer-animated films. Easily made, quite primitive films often serve valuable research activities by allowing the researcher to perceive relations that are otherwise missed. These, and somewhat better films, are used for explanatory purposes and for in-house reporting; formal reporting films require more care. Varying from primitive to "professional" quality, educational films are being used for enhancement of understanding. The quality films (and those for wide dissemination) may require very exacting attention to many detailed considerations. Cost estimates may vary from less than \$3 to more than \$3,000 per minute of screen time. The three-dollar film makers are thinking only about 16-mm film costs, while the \$3,000 film costs include many things like programming, computing time, professional film processing and editing, and studio or facility time.

Contrast control has been a long-standing problem and is often an important consideration where "grey scales" are required. Techniques and equipments are improving.

The use of color can be very helpful in delineating effects and providing information (green forests, brown deserts, blue oceans) and for readily available exposition. The "true glorious colors of nature" are very difficult to achieve, partly because of the grey level control problem which impinges upon the saturation control. The use of simple color is becoming more readily available and might be fairly easily achieved in your environment if some of the required ingredients already exist and if the demands of your requirements match these ingredients. A detailed examination is provided in "Computer Assisted Assembly and Rendering of Solids."⁴

This has not been an exhaustive review of the generation of cues — only a review of some of the more powerful ones. Examination of your particular requirements may suggest that you use more or different ones.

VII. THE ENDLESS THICKET

It is an almost irresistible impulse to make a movie when we see a computed graphic display. It should be simple. The required technology for many kinds of Kineticonics exists and continues to improve.^{5,6} I have been groping my way through the endless thicket of detailed minutia only to discover at every step that many others have previously encountered the same thorns. I am often lost in the semantic jungle that pervades the various disciplines. How do we achieve that straight path toward the bright horizons? As my daughter often reminds me, we must "communicate — brain to brain."

Let us now accept Professor Kent Wilson's⁷ challenge to "nucleate communications" and get our many colloidal talents into a cohesive coagulum of brain-to-brain understanding.

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*UAIDE (Users of Automatic Display Equipment) publishes a volume of Proceedings following each annual meeting, maintains a Micromation and Program Library, and supports three major UAIDE Committees in: Computer Animation, Scientific Systems, and Business Systems.

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DOCUMENT CONTROL DATA - R&D		
<i>(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)</i>		
1. ORIGINATING ACTIVITY (Corporate author) Lincoln Laboratory, M.I. T.	2a. REPORT SECURITY CLASSIFICATION Unclassified	2b. GROUP None
3. REPORT TITLE Kineticonics and Molecules		
4. DESCRIPTIVE NOTES (Type of report and inclusive dates) Technical Note		
5. AUTHOR(S) (Last name, first name, initial) Davis, Robert N. FitzGerald, James J.		
6. REPORT DATE 16 September 1971	7a. TOTAL NO. OF PAGES 11	7b. NO. OF REFS 7
8a. CONTRACT OR GRANT NO. F19628-70-C-0230 b. PROJECT NO. 649L c. d.	9a. ORIGINATOR'S REPORT NUMBER(S) Technical Note 1971-38	9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) ESD-TR-71-268
10. AVAILABILITY/LIMITATION NOTICES Approved for public release; distribution unlimited.		
11. SUPPLEMENTARY NOTES None	12. SPONSORING MILITARY ACTIVITY Air Force Systems Command, USAF	
13. ABSTRACT Evolution of the ability to compute molecular models inevitably leads to exploration of the ways in which models may be converted from computed bits and bytes into readily perceivable mental imagery. Computer-generated dynamic graphic methods may be used to provide enhanced understanding for research, technical reporting, technical explanations, and education.		
14. KEY WORDS dynamic computer graphics chemistry education technical artistry molecular motion		