Computer Films: Adding an Extra Dimension to Research

Only a few who attended the recent AAAS annual meeting witnessed an extraordinary demonstration of the power of animated computer films. Picture a sphere with its familiar grid of lines of longitude and latitude. The sphere begins to change shape, and, gliding from one contorted configuration to another, ultimately ends up turning itself inside out before returning to its original position—all in vivid color and to the tune of an eerily futuristic musical score. This short film probably taught viewers more about the differential topology of three-dimensional surfaces than any number of drawings in books. If, as the old saying goes, one picture is worth a thousand words, then for some researchers one movie is worth a thousand pictures.

But, considering the age of computer film making—it had its beginnings in the mid-1950's—researchers are hardly flocking to use the technique. In part, the dearth of activity has been due to the expense of making films, which demands considerable investment both in hardware and in the development of computer programs. Contributing to the problem has been the unavailability of standardized computer programs of the type needed to generate the computer graphics displays that are sequentially photographed in the film-making process. Nonetheless, there has been an increasing interest in computer films among chemists and physicists as they try to extract more and more information from increasingly realistic models of complicated phenomena.

A recent meeting* sponsored by the American Physical Society provided an opportunity to survey some of the ways investigators are using computer films to aid their research. One auspicious outcome of the get-together is that film makers are going to try to make the newly opened National Resource for Computation in Chemistry (NRCC) at the Lawrence Berkeley Laboratory a repository for computer film programs and a centralized facility for making computer films that will be open to all interested users. Some participants also forecast that the ever-decreasing cost of the integrated circuits used in computer memories may help lower costs somewhat.

Computer films are an offshoot of the more inclusive field of interactive computer graphics. Interactive computer graphics usually means the display of the intermediate or final results of computer calculations, either in alphanumeric or pictorial form, on a cathode-ray tube display device. The researcher can direct the progress of a computation during execution of a program by way of a keyboard terminal, a light pen, or some other means that modifies what is shown on the display or answers questions appearing there. Although not so expensive a proposition as computer films, interactive computer graphics has been plagued by the same two problems of cost and unavailability of standardized programs, and has been "poised for takeoff" at least since 1970.

The problem addressed by the use of interactive computer graphics and computer films is the often-discussed issue of man-machine communication. For example, the computational power of computers is so great that solutions to exceedingly knotty scientific problems are too intricate to be easily understood when presented in the form of a table of numbers or even a series of graphs. In some cases, the sheer bulk of data returned by the computer is so great as to defy comprehension. In others, a person may not, at first, even have a clear idea of what is the right question to ask. The computer, in these instances, has the answer but is unable to communicate it to the researcher.

Often, the extra perspective needed to interpret the computer's results can be provided by animation. To clarify the structure of a complex molecule, it can be rotated to give the illusion of seeing it in three dimensions. The evolution of a three-dimensional surface representing the pressure in a fluid can be followed as time or some other parameter continuously changes in the computer simulation of weather patterns. Computer animation confers to the researcher what Kent Wilson of the University of California calls the extended eye; it enables a person to qualitatively see relationships that just do not show up in static pictures.

Richard Miller of the University of Chicago, for example, makes more than 50 computer films during the course of a year in his experiments on the dynamics of galaxies. A typical galaxy may contain 10^{11} to 10^{12} stars (or, as Miller quipped, a number about equal to the dollar amount of the Defense Department's annual budget), each of which interacts gravitationally with all the others. The only way to study the time evolution of such a complex system is by way of computer modeling. In this way, the answers can be found to such questions as what happens to the assembly of stars over a period of several hundred million years, and does the computer simulation reproduce any observed features of the structure of galaxies?

In one such simulation, carried out at the National Aeronautics and Space Administration's Ames Research Center, involving 115,000 stars initially in a uniform distribution, Miller found two unexpected structures developing with time. The first consisted of two parallel sheets of stars, but it soon (on a galactic time scale!) dissipated. Later on, a bar-shaped configuration that rotated end over end took form. This second structure did not fall apart, at least over the time of the simulation. The first configuration corresponds to no observed galaxy, but the tumbling bar may be related to real galaxies having the so-called barred spiral structure and to certain elliptical galaxies.

Miller emphasized in his presentation that, since these structures were not anticipated, there would have been little chance of finding either without the animation provided by the computer films. Moreover, the compositions of the structures constantly changed (that is, stars entered and left), although the overall shapes did not, a dynamic feature not easily detected without animation.

In many instances, the effect of the insight gained from viewing a computer film is less a matter of getting a final answer than a matter of discovering what the essential features of an otherwise hopelessly complex situation are. The benefit is thus in knowing where next to spend one's computational dollar to get the most information. Consider collisions between molecules that sometimes lead to a chemical reaction and other times give no reaction. As the total number of atoms in the molecules increases beyond a few, calculation of when and how reactions occur rapidly becomes, if not an intractable, a highly involved

*Symposium on Computer Films for Research in Physics and Chemistry, Joint Institute for Laboratory Astrophysics, Boulder, Colorado, 20 to 22 March 1978. A film composed of clips from state of the art efforts shown at the meeting is to be produced for the Chemistry Division of the National Science Foundation and will serve as the symposium proceedings.

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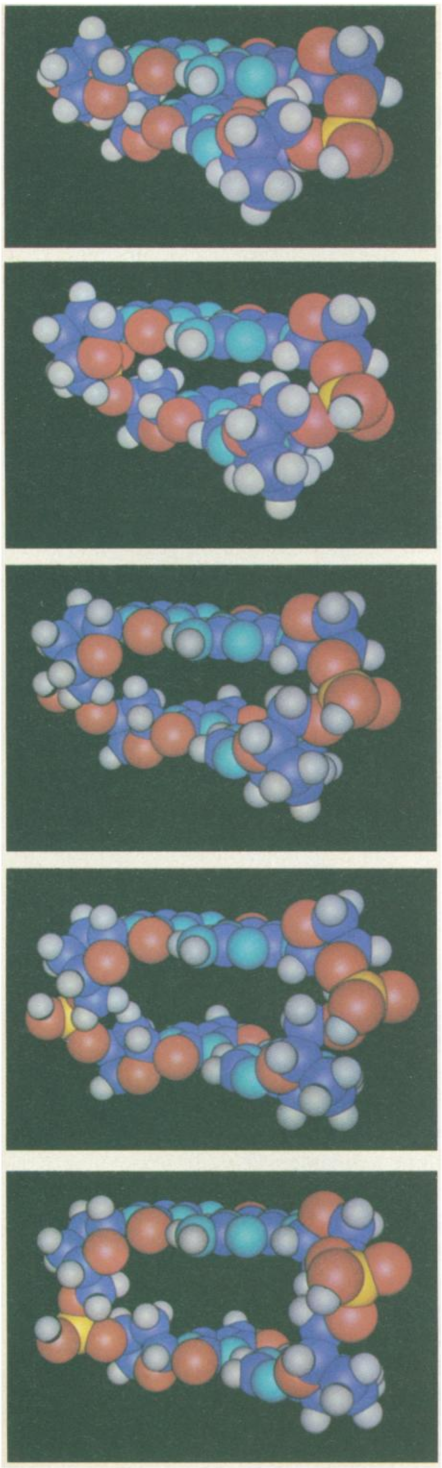

proposition. Computer simulations of such collisions have helped Charlotte Slater and the late Don Bunker of the University of California at Riverside and Trina Valencich of the California State University at Los Angeles sort through the myriad ways methane molecules and isotopes of hydrogen can interact, a six-atom problem.

The difficulty comes with the necessity, in the absence of prior knowledge, of calculating the probability of a reaction occurring for all allowed combinations of initial velocities, orientations, and impact parameters of the molecules, although only a small fraction of these combinations are "interesting"—that is, lead to a reaction by one of several possible mechanisms. The role of the computer simulations is to find these interesting combinations by way of a Monte Carlo (random) sampling technique.

Valencich showed computer films of a few of the 20,000 or so molecular trajectories (not all of which are filmed) computed from the randomly selected initial conditions. The filmed trajectories, made in collaboration with Herbert Bernstein and James Muckermann of the Brookhaven National Laboratory, graphically illustrate the paths, changes in orientation, and exchanges of atoms (if a reaction takes place) between molecules as collisions or near collisions occur. In this respect alone, the films are highly instructive. The real virtue of the films, however, is that the researcher can quickly see that certain combinations of velocities and positions do not come remotely close to leading to a reaction. Thus, further attention to these or similar configurations can be dispensed with and detailed calculations can be concentrated elsewhere. A second advantage is that unexpected events can be located and selected for closer inspection. For example, a particular set of initial conditions was found to give rise to a collision

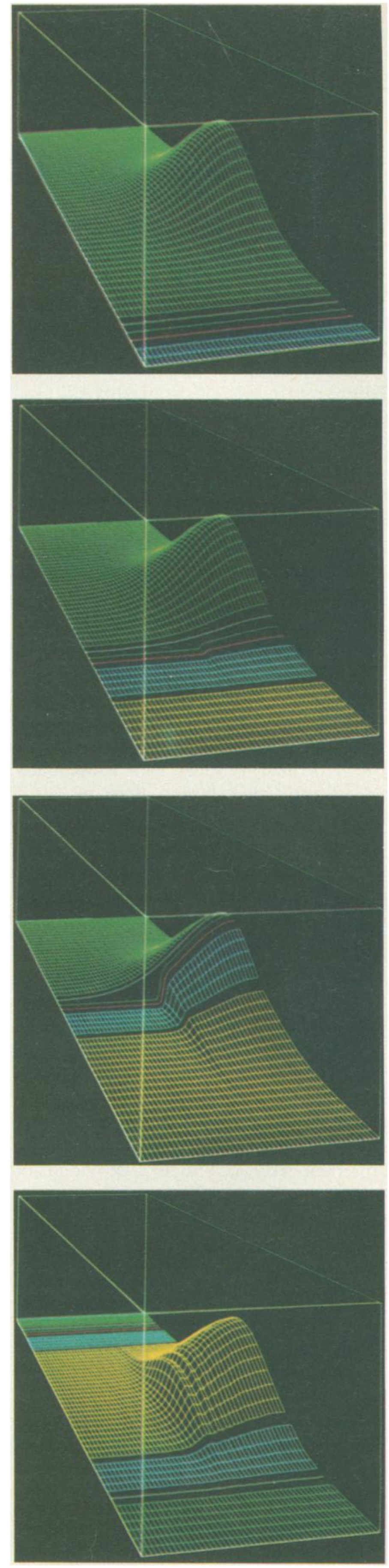

Fig. 1. Sequence showing, for a portion of a DNA molecule, the change in conformation as the distance between two neighboring base pairs increases from the normal 3.38 angstroms to about twice this separation. The base pairs lie in the horizontal planes connected by phosphate and sugar groups, which constitute the backbone of the helical DNA molecule, on the left and right. (The color scheme: red, oxygen; yellow, phosphorus; light blue, nitrogen; dark blue, carbon; and white, hydrogen.) Each view of the molecule took only 2 seconds to calculate on a high-speed maxicomputer, while the shading and highlighting routine required 4 minutes per 2048 by 2048 element color picture on a computer output microfilm recorder driven by a minicomputer. [Source: Nelson Max, Lawrence Livermore Laboratory]

Fig. 2 (right). Sequence illustrating passage of a laser pulse through a carbon dioxide laser amplifier. The amplifier consists of four stages, each of which comprises the optically active carbon dioxide gas (yellow) where amplification takes place, sulfur hexafluoride "absorber" gas (blue) whose purpose is to prevent unwanted lasing before the main part of the pulse arrives, windows between the exterior air gaps (green) and the interiors of the amplifier stages, and an aperture (red). Shown is the partial deterioration of a pulse after passage through the first stage due to diffraction effects at the aperture. The vertical coordinate is the amplitude of the electric field in the laser pulse, and the horizontal coordinate is the radial distance from the axis of the laser system. The third coordinate is the position of the pulse along the optical path, but the animation is designed so that the pulse always sits in the center of the box and it is the laser system that flows through. [Source: Donald Dickman, Los Alamos Scientific Laboratory] geometry previously not thought to lead to a reaction. In the simulation, however, a reaction was produced.

With high performance computers, large computer memories, and interactive graphics terminals, it is possible to achieve animation in "real time" on the display screen without resorting to filming. This practice is already widespread—in industry as well as academe—and is being used in connection with simulators for training pilots to land aircraft, the design of automobiles, the analysis of high energy physics data, and the construction of models of complex biological molecules. In applications where extensive computation must be done between "frames," however, animation is not possible in "real time" but becomes possible only after each frame is computed and filmed. Similarly, the large amount of information needed to generate television-like (raster scan in which every one of about a million elements in the matrix making up a picture must be specified) images makes real time animation of these not feasible. [It is the simpler stick and ball (vector scan in which only the start and end points and the type of figure need be given) images that can be manipulated in real time.] Although the interactive capability is lost in these cases, the advantage of a permanent record of the animated sequence is gained.

A Useful Teaching Device

A use for which the permanent record capability of computer films is especially useful is a didactic one. Scientists can sometimes do a much better job of explaining their research to others, whether to a specialized or to a lay audience, by way of an animated film. Especially important classes of viewers are the laboratory manager and the contract or grant officer of a funding agency, and more than one film maker reported positive results after a film showing.

A more serious example perhaps is classroom instruction; students are both more interested in and more able to grasp complex concepts when they are presented by way of a film. The power of films, at least as an attention-getting device, was amply demonstrated at the meeting when a nighttime showing of a movie on computer animated chemistry by Kent Wilson drew a nearly packed house during mid-term exam week at the University of Colorado. Similarly, a showing of three-dimensional computer films by R. S. Hotchkiss of the Los Alamos Scientific Laboratory required a second screening when interested students took so many seats that not all conference attendees could view the film.

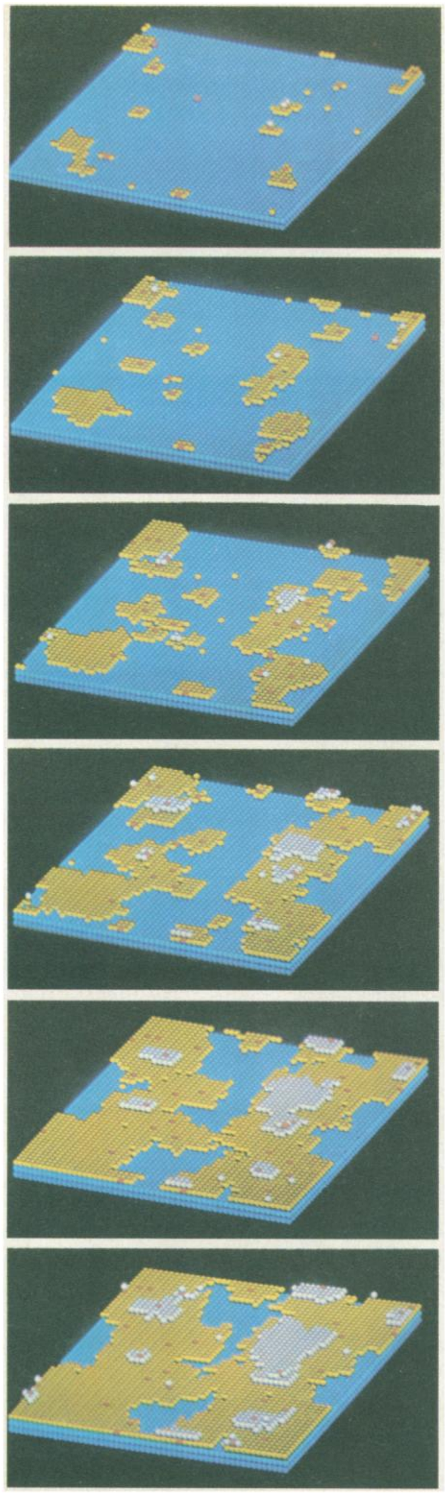

Fig. 3. Sequence showing how crystal growth is enhanced by the presence of impurities. Atoms arriving at the surface from the vapor may stick there and remain in place or move about. When impurities bond strongly to the host atoms, crystal growth tends to occur by nucleation of clusters of host atoms around the impurities with consequent spreading of the clusters until they meet and a complete layer of atoms is formed. Under conditions favorable to cluster formation, new clusters can form on partially completed layers even before they are completed. Blue atoms are those forming the substrate, yellow atoms belong to the first layer above the substrate, and white are in the second layer above. Red atoms are the impurities. [Source: George Gilmer, Bell Laboratories]

According to Ken Knowlton of Bell Laboratories, computer film making for research began about 1956 when a few individuals at institutions—such as Bell Labs, the Boeing Company, the Massachusetts Institute of Technology's Lincoln Laboratory, and the Lawrence Livermore Laboratory—that had high performance computers and some sort of visual display device independently conceived the idea that certain problems that could be defined mathematically might be more easily attacked by computer animation, especially when there was no clear indication of what their solutions would look like. The first films were crude by commercial standards; but as the years went by, sound tracks were added and color became available. Today the best films perhaps still do not rival Walt Disney, but they are closing the gap. A film by Nelson Max of Livermore, showing the structure of a portion of a DNA molecule, was probably the most polished example of the state of the art at the conference (Fig. 1).

Turning On with Color

Anton Hopfinger and Deepak Malhotra of Case Western Reserve University are collaborating on a project to calculate the conformations of various drug-DNA complexes. The expectation is that some of the conformations found will lead to models of how mutagenic substances can disrupt DNA molecules and thereby cause mutations, but the project is still in its beginning phase. Using a computer program developed by Lorinda Cherry and Knowlton of Bell Labs and the Case Western calculations, Max made a color computer film that examined changes in DNA conformation that were brought about by increasing the spacing between neighboring base pairs. At this early stage of the project, the film could not convey much new information and was mainly an exhibition of technological virtuosity; but the model of the molecule, rotating and changing its shape, with the addition of shading and highlighting to provide additional three-dimensional effects, drew audible gasps from the audience.

Color, in fact, is turning out to be more an essential than a frivolous ingredient of films because its use permits the display of more information than black and white alone. Donald Dickman of Los Alamos showed, for example, a computer simulation, made in collaboration with John Goldstein, of the passage of a high-power light pulse through the optical system of a laser being developed for fusion energy reactors. This particular example further illustrates the usefulness of computer simulation in the absence of experiments that can provide the information needed. In the case of the high-power laser, the problem is how to design the optical system so that the laser pulse retains its shape well enough to be focused onto the tiny microballoons filled with deuterium and tritium that serve as the fuel in laser fusion reactor schemes. In particular, diffraction effects tend to destroy the quality of the pulse, but how to cure them was not discovered until computer simulation was carried out. From the information gained in the simulations, it was possible to redesign the apertures that shape the laser pulse to minimize the diffraction.

The computer film was made in such a way that the viewer "rode" the pulse through the laser system and thereby monitored the change in the shape of the pulse as it sped along its path. Since the laser system consists of several components that are repeated four times in a particular sequence along the path, it was by means of color that the cause of the diffraction could best be localized. This was achieved by changing the color of the coordinate system as the laser pulse entered each new region of the system, so that the viewer could see where the pulse was by its color (Fig. 2).

A similar use of color was made by George Gilmer of Bell Laboratories in his animated simulations of crystal growth. Each layer of the crystal was a different color—as were impurity atoms, if present. In one case, the use of color helped illustrate the role of impurity atoms as nucleation centers for the growth of clusters of atoms on a surface (Fig. 3). Gilmer pointed out that another role of the film was one of enhancing the quality of the communication between theorists and experimentalists in the field of crystal growth, as the two groups of researchers apparently operate on different wavelengths much of the time.

More than a Camera Needed

How is a computer film made? The naive way to approach film making would be simply to photograph the computer output displayed on the cathode-ray tube display of a computer graphics terminal. One problem with this method is that the resolution of most terminals is low (the picture is typically composed of a 512 by 512 square matrix of dots, or fewer). Thus, when the film is blown up on a viewing screen, effects of the low resolution such as jagged lines are easily visible and quite disturbing. More primitive, although it has been done, is to photograph, page by page, a succession of drawings generated by a plotter.

In practice, many film makers now use a device called a computer output microfilm (COM) recorder. COM's were originally designed for directly recording computer-generated alphanumeric data on microfilm at very high rates—up to 30,000 lines per minute. More recent versions find use in such applications as image processing of satellite photos of the earth. The essential ingredients of these devices are the digital electronics to convert the computer output into the signals that drive a high resolution (for example, a picture composed of a 4096 by 4096 square matrix) cathode-ray tube, focusing optics, color filters (for machines that handle color images), film for recording the image on the cathode-ray tube, and a mechanical assembly to advance the film for the next image. Crucial improvements over the early COM's that permitted viewable films included the capability of producing pictorial images as well as alphanumeric and a registration system to ensure that successive frames were aligned.

Unfortunately COM's are expensive, costing more than $200,000, according to Wayne Huelskoetter of the Dicomed Corporation, Minneapolis. (Dicomed and Information International Incorporated, Los Angeles, manufacture COM's of film-making quality.) For that reason, COM's are beyond the reach of the scientist making an occasional film. Valencich, for example, had to go to Brookhaven to find film-making equipment for her molecular dynamics simulations. Institutions that make extensive use of films are therefore the primary practitioners of the art. Livermore and its sister laboratory, Los Alamos, which do lengthy hydrodynamics simulations in their studies of laser and magnetic fusion and in weapons design, and the National Center for Atmospheric Research, Boulder, which does lengthy simulations for weather and planetary atmosphere modeling, make more films than all other institutions put together, according to George Michael of Livermore. Dickman at Los Alamos, for example, pointed out that investigators there make 100,000 feet of film each month.

Advances in electronics may help ameliorate this cost situation somewhat. For example, special computer memory devices called frame buffers, which are often used in graphics and in film making, can store the computer output needed to generate one frame of an animated sequence as it is computed for playback on a television (raster scan) screen, thus relieving the main computer of a time-consuming chore. A very sophisticated frame buffer having a picture comprising a 512 by 512 matrix and displaying up to 256 colors simultaneously was priced at about $65,000 last year, according to Ted Naanes of the Evans and Sutherland Computer Corporation, Salt Lake City. But the drastically reduced cost of the microelectronic circuits used in their manufacture means that the same frame buffer now costs 40 percent less. Some observers suggest, however, that such inexpensive devices will serve mainly to draw more researchers into the market for the more expensive COM's needed for high-quality films.

If You Don't Have Your Own COM

A second alternative is a centralized facility where researchers can go to make films. Such a center would have the equipment and a library of standard programs needed to make films. Chris Parr of the University of Texas at Dallas is spearheading a drive to make the NRCC such a center. Parr points out that the newly opened computation center's mandate easily encompasses computer film making. Moreover, says Michael at Livermore, there is a possibility that the Department of Energy's national laboratories may revive a now dormant policy of opening certain of their facilities to visiting researchers when such use would further the goals of education. If this were to occur, budding film makers would have access to a good fraction of the existing computer animation equipment in the United States.

Anyone who has seen some of the better computer films must be impressed by the spectacle, if not always the substance. But a viewer quickly amassed a list of gripes, most of which could be attributed to a lack of experience with a new medium. A particularly disturbing yet remarkably common practice among makers of color films was the use of dark red against a black background. The lack of contrast made viewing nearly impossible. In some films where time evolution of a system was portrayed, film makers did not stretch their imaginations enough and used a linear time scale even when most of the action would have been better represented, for example, by a logarithmic time scale. In a few instances, too much information was displayed at once, thus confusing the viewer more than enlightening him.

Despite lapses of these kinds, veteran practitioners of the art seem sold on the value of computer films. Although activity has somehow remained confined to a few, perhaps now conditions are ripe for a growth in computer film making.

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