Computer films for research

Movies made from the output data of complex numerical models offer perceptual advantages that can speed the recognition of unexpected behavior and encourage fruitful discussion.

John T. Scott

Let's say you have just completed a computer simulation or numerical modeling of a complex system in your physical or chemical research. The data are likely to be delivered back to you in the form of mountains of Z-fold computer printout or stacks of Calcomp plots. Rather than picking your way through all this paper, why not turn the material into a short movie that can be projected over and over again, fast or slow, to show you whatever trends, discontinuities and so on your model possesses?

Film-making from computer output is now about twenty years old. Many researchers have independently grasped its potentialities and advantages and are currently applying a variety of techniques to problems in physics, chemistry, astronomy and engineering—including such cross-disciplinary areas as biochemistry and meteorology. Some of the films have evolved naturally from experience with graphic display terminals, which provide both a familiarity with moving-image data output and the desire for high-resolution pictures that are portable and readily available for repeated showings anywhere. But other research films owe little to today's computer-graphics industry and its expensive toys; useful work can still be done with limited equipment.

The computer-movie practitioners I have talked with all emphasize the value of their films as research tools. While admitting the great value of movies as teaching aids, the film-makers whose work is quoted in this article all claim that their films are an important part of their research, sometimes showing phenomena that would become apparent from static presentations only after hours of painstaking labor—if at all.

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Film making for research passed a significant milestone in its progress toward maturity last year when the first general conference in the field took place at the Joint Institute for Laboratory Astrophysics, Boulder, Colorado. About 50 participants brought a total of around 30 movies for screening. Reflecting the unusual nature of this conference, the *Proceedings* of this APS-sponsored Symposium on Computer Films for Research in Physics and Chemistry will take the form of a series of film clips spliced together.[1]

Data explosions

It is a commonplace to say that the digital computer has triggered a data explosion in the second half of the twentieth century. But less obvious to us now is the data explosion of the eighteenth century. At that time, natural science was moving on from the largely qualitative phenomenological descriptions of, say, Michael Faraday, toward its later obsession with quantitative data. Scientists found themselves lacking a neat and concise way of presenting the numerical results of their experiments; data tabulations, already familiar from the observations of astronomers and meteorologists, were not compact and did not make clear the functional relationships between variables.

Laura Tilling has studied the early history of experimental graphs,[2] and she found that, with few exceptions, scientific observers did not plot their data in graphs before the nineteenth century. (The exceptions were meteorological data taken on automatic recorders, and James Watt's pressure–volume indicator for steam engines.) The first examples she finds are in the works of J. H. Lambert published in the 1760's and 70's. As well as drawing graphs, Lambert apparently invented the technique of determining rate-of-change by graphical differentiation.

As was often the case with Lambert's work, his contemporaries overlooked the possibilities of his innovation, and it was not until the publications eighty years later by J. D. Forbes, professor of natural philosophy at Edinburgh University, that the technique re-appeared. Forbes, in the 1840's and 50's, drew many graphs in which he would compare experimental points with suspected theoretical relationships by plotting the two together. Even his first published graph (on hourly variation of atmospheric pressure with latitude, 1834) includes a theoretical curve matched to the observations by the method of least squares. After Forbes, science has not looked back; two-dimensional graphs, on Cartesian or special coordinates, have since become the accepted way of presenting experimental data.

I have digressed into this eighteenth-century problem because I see useful parallels between the invention of experimental graphs and the use of computer films in research. In her paper[2] Tilling wrote:

> "The graphical representation of experimental data in the physical sciences has several advantages which today are too familiar to require very detailed enumeration. Its greatest strength lies in the clarity and succinctness with which it displays the information contained in the tabulated results: for the experimenter a graph provides a rough and immediate check on the accuracy and suitability of the methods he is using, and for the reader of a scientific report it may convey in a few seconds information that could only be gleaned from a table of measurements by hours of close study."

Read those lines again, substituting "films" for "graphs," "viewer" for "reader," and you will have an excellent description of the power of movies in research.

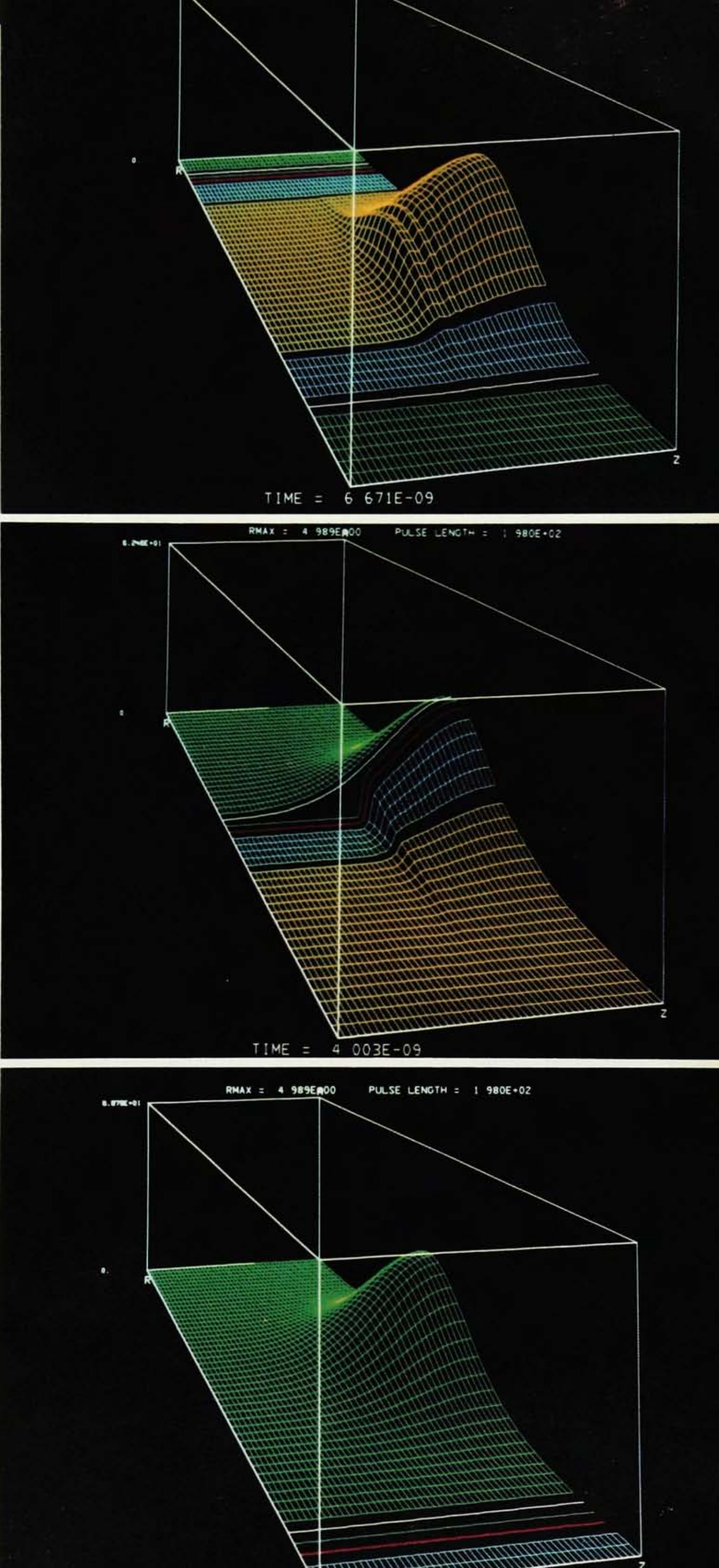
Just as graphs represent a break from the one-dimensional world of tabular columns of numbers to the two dimensions of plotted curves and areas, so do movies add a new dimension, that of time. Three-dimensional surfaces may be represented on paper by isometric projection (as in the familiar orthogonal x-y-z coordinate system); the same technique is applicable in movies to present the effect of four dimensions (x-y-z-t). What is more, the perceptual leap associated with a stereoscopic binocular view is also available in movie form, as an experimental film shown at the Boulder symposium attests.

Color, yet another "dimension," has not been greatly exploited on graphs. Movie makers on the other hand have reacted enthusiastically to the possibilities of color, to the extent that their products are not only packed with information but are also often beautiful in their own right. In this category I would place the work of Nelson Max of Lawrence Livermore Laboratory, whose DNA molecule appears on the cover of this issue of PHYSICS TODAY, and that of Donald Dickman and John Goldstein of Los Alamos, whose model of a laser pulse in a CO_2 laser amplifier is shown in figure 1.

Pedagogy or research?

Many scientists who make movies as an integral part of their research take pains to disassociate themselves from the makers of purely educational films. After all, they say, films have been used in teaching for a long time now; you don't even need a computer to plot curves when an artist can produce a convincing copy, suppressing confusing and extraneous matter in order to concentrate on the pedagogical point in question. The central difference appears to be that a pedagogical movie starts with a concept—a "shooting-script" if you like—and proceeds to illustrate it; a research movie in principle develops its own concept as it grows.

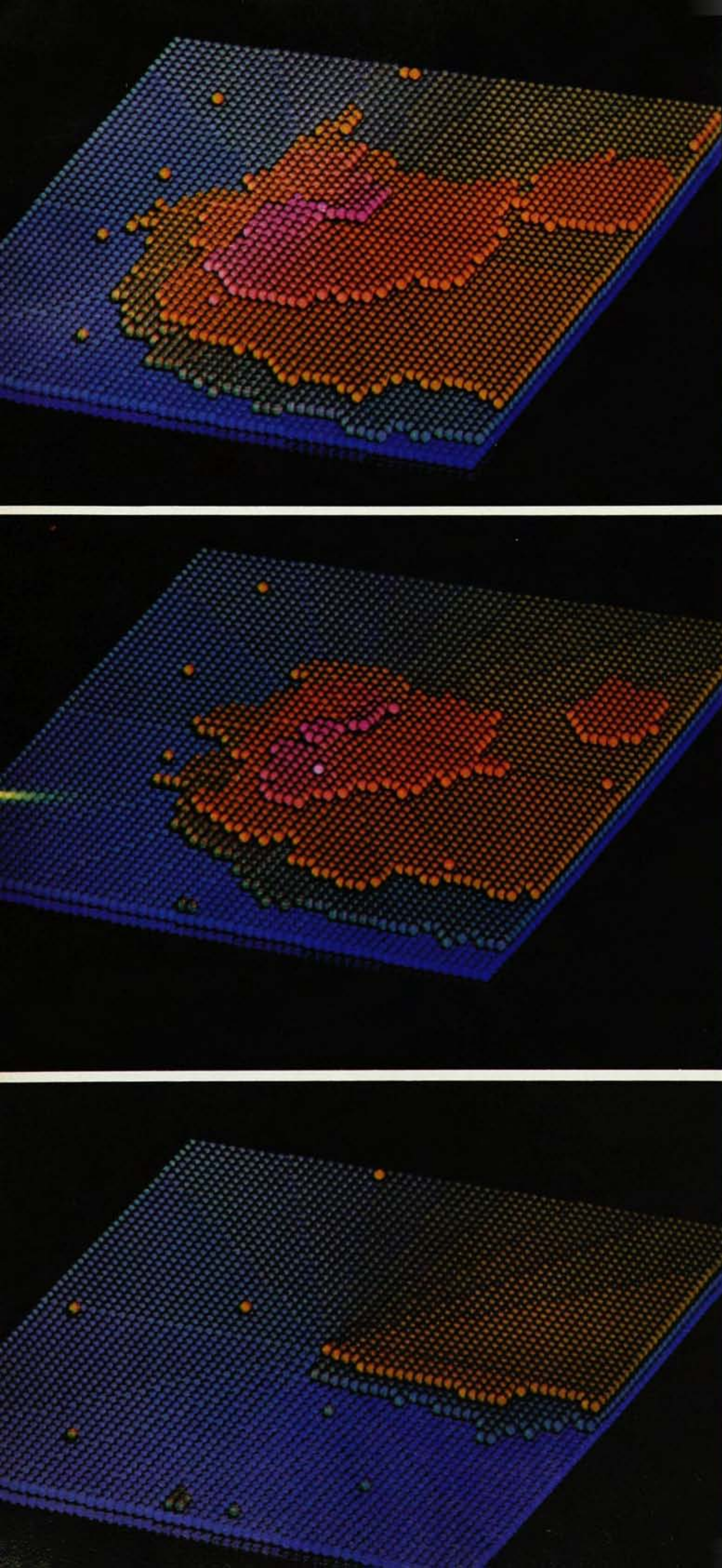
The difference is not as clear-cut in practice. Some pedagogy is present in all research films, even if limited to a showing of the movie to a handful of its author's



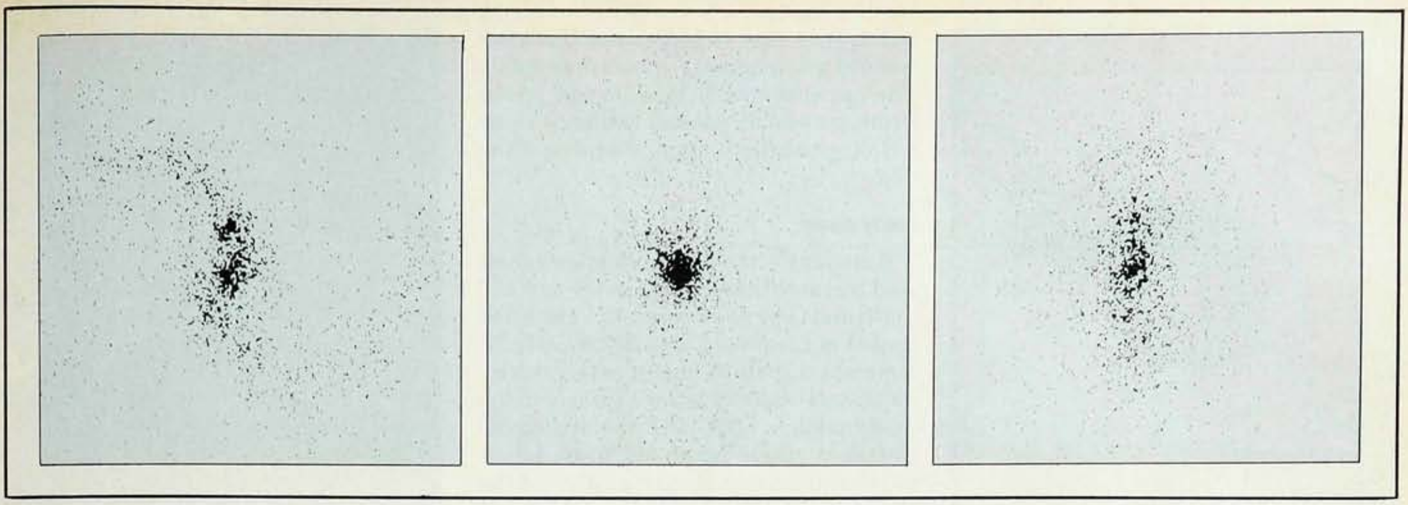
A carbon-dioxide laser pulse propagating through a four-stage system, visualized in three frames from a movie simulation by Donald Dickman and John Goldstein of Los Alamos. The view is seen through a calculational "window" that moves with the pulse, so the various media of the laser system appear to flow through the pulse as it propagates down the amplifier chain. Green represents air gaps; blue, absorbing areas; yellow, the pumped CO_2 amplifier, and the red line is an aperture. The scale of the vertical coordinate is continuously adjusted to normalize the pulse height. Figure 1 colleagues to generate discussion and advice. Closely related to education is the use of movies in public-relations activities and for presentations to funding agencies. I understand that at several laboratories well-produced, colorful movies have played successful roles when the agencies asked for a progress report at grant-renewal time!

Joe Eberly of the University of Rochester (and one of the organizers of the JILA symposium during his visiting fellowship there) commented to me on the justification for spending time and money "merely" to make movies. He believes that movies should be seen as a scientific tool for discovery, not measurement. "It seems to me," Eberly continued, "that most scientists make measurements, not discoveries. This is, perhaps, obviously true of experimentalists, but I think equally true of theorists, who mostly make calculations within well-defined limits; that is, they measure the consistency and range of a given theory. Scientists in general are certainly more comfortable with measurement than discovery. Discovery is always an inefficient and haphazard enterprise, and usually expensive. Most scientific tools are designed for measurement, and very few specifically for discovery." So, Eberly concluded, it is not surprising that some research movie-makers are still disturbed "because movies don't, can't, measure anything."

Movies do, however, discover things. An example is in the work of George Gilmer and Ken Knowlton of Bell Labs, some stills of which appear in figure 2. Gilmer and Knowlton use movies to explore the unexpected features of crystal-growth models being developed by Gilmer and John Weeks.[3] For their calculations they find the kinetic Ising (or lattice-gas) model of the crystal-vapor interface the most useful; it provides an atomic-scale representation of the growing crystal, including processes of condensation, evaporation and surface migration. This model is also well-suited for computer-simulation "experiments," carried out with a Monte Carlo statistical technique. Movies of the computer simulation, with atoms in adjacent crystal layers colored differently to allow the observer to distinguish one from another, are fascinating to watch. All the processes listed above can be demonstrated, as can others such as the effect of adding impurity atoms. Particularly impressive is the sequence



Spiral growth at a screw dislocation; three frames from a movie by George Gilmer and Ken Knowlton of Bell Labs. Time progresses from the bottom frame upwards. This simulation explores crystal-growth models by Gilmer and John Weeks that study the crystal–vapor interface, by Monte Carlo calculations, in the kinetic Ising formulation. The process can be repeated for any combination of temperature, interatomic potentials, deposition rate and so on. Its authors credit the movie with detecting a hitherto unsuspected singularity in the Ising model as used in this calculation. Figure 2



Three-dimensional self-consistent model of an initially spherical rotating galaxy. These are orthogonal views of a 115 000-particle "galaxy" at one instant during its development in a calculation by Richard H. Miller, carried out on the ILLIAC-IV computer at NASA Ames Research Center. The S-shape visible here (in the view on the left) is not stable; the galaxy eventually settles down to a barlike form. Figure 3

(figure 2) that shows spiral growth at a screw dislocation. Model experiments include the effects of changing temperature, interatomic potentials, deposition rate and so on. Gilmer points out the great value of these movies as a bridge for communication between theorists and experimenters, and as a way to stimulate discussion and guide future work.

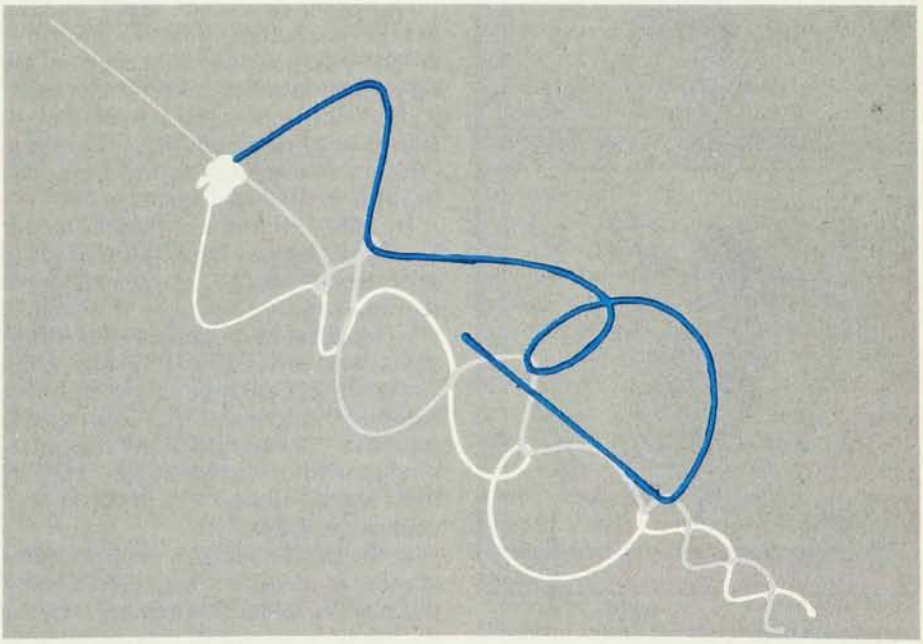
Discoveries made as a result of this movie-making project include new knowledge about the effect of impurities and of defects on crystal growth, and the identification of a previously unsuspected singularity in the Ising model. This information was in principle available from the computer calculations alone, but Gilmer and Knowlton both praise the movie approach highly as an indispensable aid.

Richard H. Miller of the University of Chicago claims that his discovery of unexpected behavior in rotating galaxies could only have been made by making and viewing films. Miller, using the facilities of NASA's Ames Research Center, makes large n-body calculations containing up to 115 000 particles representing an initially spherical galaxy.[4] As the rotating system evolves in time, unsuspected patterns grow and disappear; at one stage the "stars" tend to form two parallel sheets. The galaxy eventually settles down with a cigar-shaped cluster at its center (figure 3). No spiral galaxies are stable in this model. Miller suspects that many of the familiar elliptical galaxies have this prolate spheroidal shape rather than the oblate spheroidal (disc-like) shape that has usually been assumed. His films show clearly that it is the geometrical forms that are stable, not particle orbits; "stars" are continually entering and leaving the central cluster but with statistical frequency such that the form itself is undisturbed.

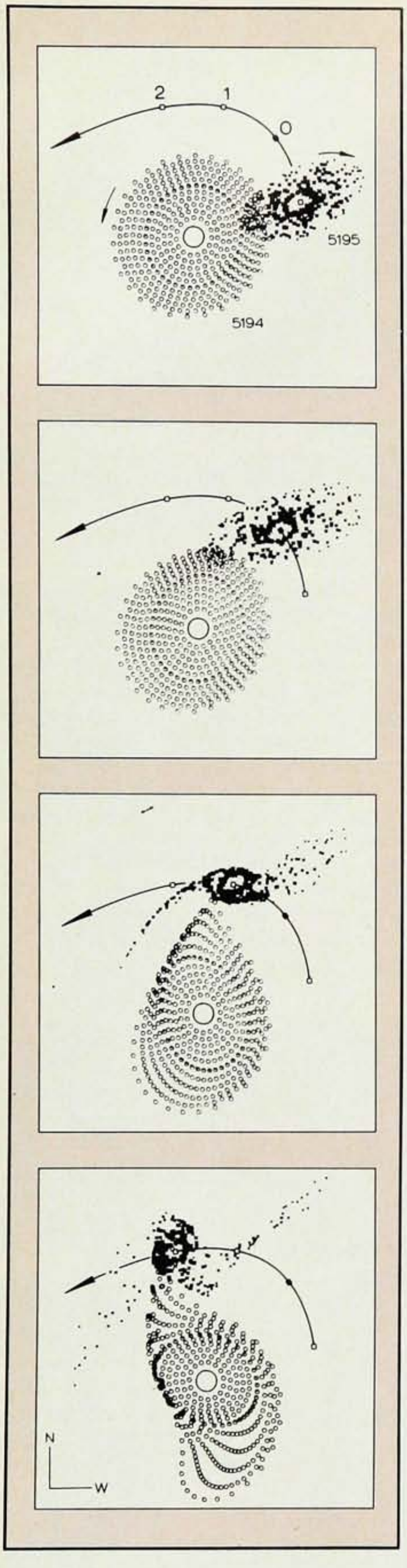
All the movies presented at the Boulder symposium serve to emphasize the points I have made with the preceding two examples; their strength lies in the higher level of human perception brought to bear on them, as compared with other forms of presentation, and the greater insights that then become available. Some movies are only viewed by their authors, seeking help for model-fitting. Many of these are discarded, having served their purpose. The films that are eventually shown to large and appreciative audiences represent the result of that development, and the pedagogical element comes to the fore when the researcher explains what he has been doing and points out interesting features of his film.

Likewise the necessity for expending time and money on the movie may not be apparent when, in a publication such as this article, the text is necessarily illustrated with selected stills or short sequences taken from the film. When you look at the illustrations on these pages remember that, self-sufficient though some of them appear, in each case their significance was realized in the context of the original movie.

One danger I see in the proliferation of computer films as research aids stems from their very persuasiveness. When you look at the Bell Labs crystal models, with atoms floating down from above and nestling onto the lattice, or when you view Miller's slowly rotating galaxy forming and reforming complex shapes in its in-



An astronomical three-body collision calculated and illustrated by Leigh Palmer of Simon Fraser University. In Palmer's movie the three objects appear as moving white dots; for this illustration the entire track length has been drawn in to provide a history of all three paths. The event starts with a binary system (white blob near upper left) and a third object approaching from the upper left corner. Most of the middle of this figure is occupied with the convoluted paths of the three objects immediately after collision. Finally, two of the objects move off screen at the lower right as a new binary system, while the third leaves in the opposite direction. Figure 4



A tidal encounter between galaxies. Alar and Juri Toomre model the perceived structure of NGC 5194/5 as an interaction between previously independent galaxies (top frame), reproducing the present appearance (bottom frame). The four frames reproduced here show the encounter as seen from the Sun; the complete calculation includes an orthogonal view as seen by an observer to the west. Figure 5

terior, it is easy to forget that the phenomena you see are still model dependent. The suspension of disbelief can be just as strong as when a general audience views a Hollywood production of a piece of fiction.

Early days

Apparently the first computer-generated research movies were made by Cecil Leith and George Michael on a classified project at Livermore, around 1956. Leith remembers these as being "pretty crude" black-and-white films on a subject in hydrodynamics. By 1961 the first non-classified movie appeared from Livermore; this was on Leith's model for the global circulation of the atmosphere. It also had the distinction of being the first computer movie in color (produced from three black-and-white films printed as a color composite). During the mid-1960's the recently created National Center for Atmospheric Research was working on its own global-circulation model, and Warren Washington began making computer movies, in color, of this model.

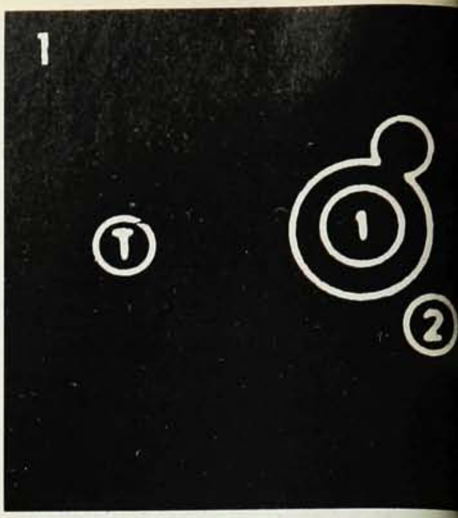
The early NCAR movies of atmospheric circulation patterns are still eminently viewable, though primitive by today's standards. In particular, the accompanying commentary to these silent films was handled unsuccessfully (a long written explanation, typed white-on-black, scrolls hypnotically up the screen). Later examples, of course, are sound films with voice-over narration. Since this early start, Livermore and NCAR have continued making computer movies, both now ranking among the leaders in technique and output.

Computer-produced movie-making became available to all, in principle, around 1960 with the manufacture of the computer-controlled microfilm recorder. This device is intended for permanent, high-density data encoding onto microfilm, but with appropriate software it can be made to produce 16-mm movies.

By 1967 the National Committee for Electrical Engineering Films was able to produce a 20-minute "interim report" on movies from computers in the form of clips from the best examples then available. And in 1971 Kent Wilson of the University of California at San Diego put together "Patchwork '71," a 20-minute collection of excerpts from computer-produced films in chemistry. Most of these earlier movies were made for educational purposes.

In the last ten years an ever-increasing number of physicists and chemists have taken up computer film making. Among the factors responsible for the increase are:

- The cost of computing time has moved dramatically downward
- Excellent film-making equipment, concentrated at several large computing centers, is now available
- Some researchers have found inexpensive short-cut techniques for making movies of at least an adequate standard.

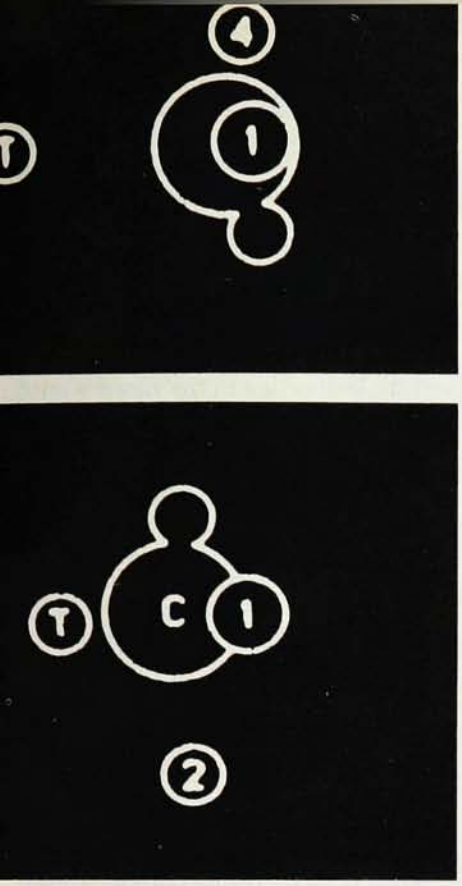


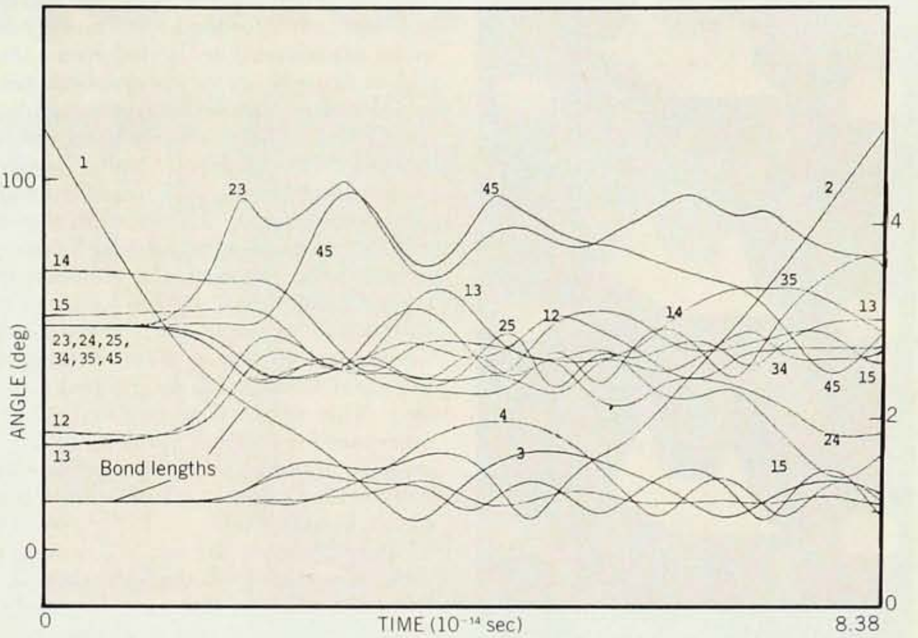
A molecular collision involving six atoms. This is an example drawn from the work of Trina Valencich and her colleagues, in this case for the process $D + CH_4 \rightarrow H + CH_3D$. All the data from the calculation are present in the bond-length and bond-angle plots shown in part a of the figure (on the far right); but visualization of the collision is virtually impossible without the movie (three frames, above and immediate right, constitute part b of the figure). The incoming atom is labelled "T"; the four hydrogen atoms are identified by the numbers 1 through 4, and "C," of course, is the carbon atom. Figure 6

Techniques

Computer-animation techniques are by now well established. For many years, design engineers and architects have been able to select library programs for rotation and magnification of images drawn in perspective on their interactive video display terminals, and the software includes such features as "hidden-line" removal, and shadows and highlights on the representation of solid objects. Computer animation can also be seen on most TV stations' identification logos.

Many of these techniques can be utilized for research films. The quality of the results can be judged from the example on the cover of this issue of PHYSICS TODAY. Produced by Nelson Max of Livermore, in collaboration with Anton Hopfinger and Deepak Malhotra of Case Western Research, it shows a portion of the DNA molecule. In the movie from which this still was taken the molecule apparently rotates in space before the observer, so allowing a complete three-dimensional examination of its structure; then the DNA base planes increase their separation and the attached groups rotate to take up a new configuration. The programming necessary to produce this display is based on a software package written by Ken Knowlton and Lorinda Cherry of Bell Labs called ATOMS. Max provided additional shading and highlights. Each frame contains 2048 × 2048 picture elements.





Films of this high quality must be produced by computer-driven microfilm recorder, plus whatever computer power is needed for the original model calculation. This is an expensive proposition; the microfilm recorder alone would cost you \$200 000 if you insisted on having your own. But acceptable movies can be made much more cheaply, as Leigh Palmer of Simon Fraser University has shown.

Palmer studies solar-system celestial mechanics, and he became interested in the gravitational three-body problem. Despite the well-known difficulty of this problem in the general case, special cases with defined initial constraints are easily tractable with modern digital techniques. However, the solutions are not readily understood *via* the traditional data-presentation methods, and Palmer makes movies to illustrate the simultaneous motion of the three bodies. He films directly off the screen of a Tektronix 4013 graphic storage terminal, using a Bolex 16-mm cine camera and Plus X film. The camera shoots single frames from the screen, and its frame-advance motor is controlled by a microphone that picks up the sound of the bell on the Tektronix. All the equipment is portable, and both terminal and camera can be released to other users at short notice.

Palmer's movies are particularly difficult to illustrate with stills, such as those in figure 4 which are from a film he made of a three-body gravitational system. For these stills the terminal operates in its storage-display mode, so that the moving bodies (here assumed to be stars or comets) leave trails to show where they have been. It is just possible to pick out the trail of the incoming object, the confused trails as the two originally orbiting bodies of a binary system fly apart, and the final condition where the captured body settles down with one of the others and the pair move off the screen together, leaving the third behind. But the stills are no substitute for a viewing of the movie, where the three trajectories can be followed in detail while the objects perform their stately dance.

Movies can be immeasurably improved with the addition of color and sound—color to separate otherwise confusing details, sound primarily to provide a commentary. Many of the more sophisticated modern examples have a music track as well. These extra features, however, are intended only to increase the film's appeal to a general audience; if the intention is to make a research movie primarily for private consumption, silent black-and-white is satisfactory. If you *do* intend to add color and sound to a movie, though, it pays to get expert advice. The techniques are simple enough but conceptual errors are frequently made by the inexperienced.

I asked several film makers if they had considered videotape as a substitute for film. After all, the data are originally digitized; surely they could be transferred easily to videotape directly from the computer? The universal choice of 16-mm film appears to be due to the excellent resolution possible in this medium, and to the ready availability of projection equipment for screening away from the home laboratory.

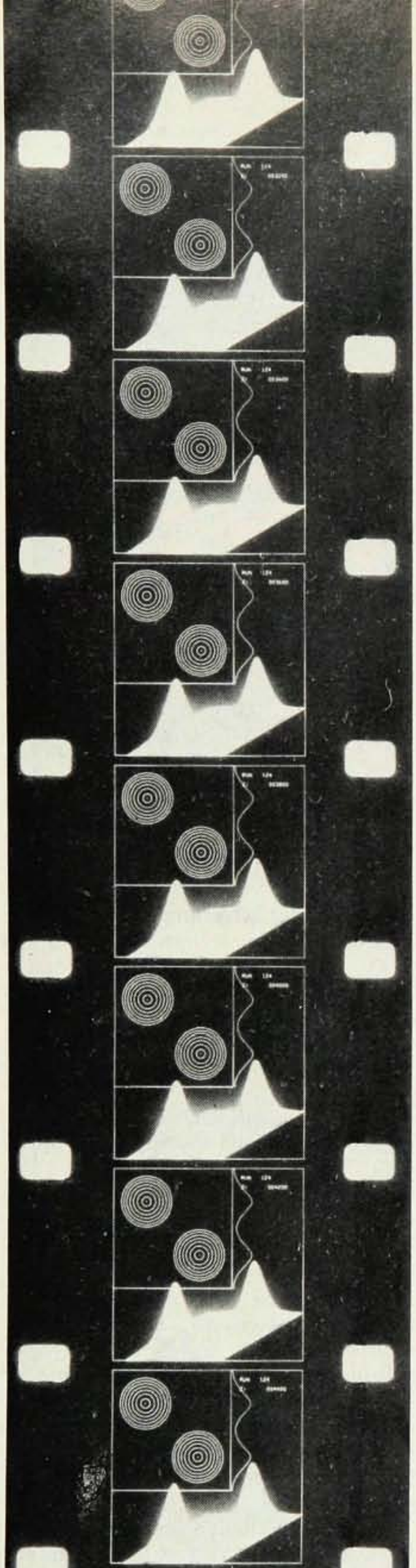
Range of subjects

What projects make the most useful computer films? The movies I have seen group themselves into three major categories:

- Particles moving in three-dimensional space, constrained by specified force laws
- Animations of complex shapes
- Planar curves changing with time, and three-dimensional surfaces changing with time.

Examples of the first category are found in astronomy, chemistry and solid-state physics. We have already seen astronomical examples by Miller and by Palmer; another example is the work of Alar and Juri Toomre of MIT and JILA respectively. Typical of their films is the sequence shown in figure 5. This is a calculation of tidal damage in the "Whirlpool" double galaxy, M51 + NGC 5195. The view is that of an observer on Earth, and the frames show damage to the outer parts of both galaxies, presumed to be the eventual result of the interaction.

In this category, an example from solid-state physics is the Bell Labs crystal-growth work mentioned earlier. An example from chemistry is the series of movies made by Trina Valencich of California State University at Los Angeles. Using Brookhaven facilities and Herb Bernstein's adaptation of an Oak Ridge program, she and Jim Muckermann have



Self-focussing in a laser beam propagating in a nonlinear dielectric medium. Each frame of Frederick Tappert's movie includes a contemporaneous intensity curve and spectrum in one dimension and a contour plot and a surface plot in two dimensions. The results yield information about breakup and filamentation of high-power beams. Figure 7

shot films of molecular-collision dynamics, including systems as complex as[5]

$$D + CH_4 \rightarrow H + CH_3D$$

Orbits of all six particles are calculated, and the data can be represented in the bond-length and bond-angle plots against time, figure 6a. But the additional degree of perception afforded by the movie has to be experienced to be believed—the stills in figure 6b are very poor substitutes. In the movie, the incoming atom glides toward the molecule (drawn in true perspective); the molecule waits, gently bobbing and pulsing with rotational and vibrational energy. Then the interloper closes in, the bobbing and pulsing increase in vigor while the newcomer seeks a way in, and finally (for a capture collision) it nestles into place and one of the original "molecular" hydrogen atoms is pushed away and moves off in disgruntled fashion. This scenario is repeated many times over for different initial conditions: angle of approach of the projectile; velocity of the projectile; temperature of the molecule, and so on.

My second category consists of representations of complex shapes in three dimensions. Max's cover picture of the DNA molecule is in this group; also representing the category are several biochemical movies made by Kent Wilson. Also by Max is a truly remarkable demonstration of the inversion of a sphere—how to turn a sphere inside out without tearing or creasing it. The full solution to this problem is inaccessible to all except those with the skill to follow the topological mathematics in which it is phrased; on watching the movie, however, anyone can (almost) see how it is done. In all these examples the value of the movie lies in allowing a close examination of a complex shape at close quarters and from all angles—like holding a model in your hands. But unlike a physical model, the scale can be dramatically changed at will, or you can make yourself small and go *inside* the object (as in a movie by Wilson of the human brain).

The third category of computer films is the largest—those in which time is an extra dimension, an extra variable to the two of a planar graph or the three of a surface drawn in projection. We have seen an example in figure 1, Dickman and Goldstein's CO_2 laser pulses. This Los Alamos film shows a simulation of a pulse propagating through a four-stage amplifier system.[6] The view is seen through a calculational "window" that moves with the pulse, so that the various media of the system appear to flow through the pulse as it propagates down the amplifier chain. The scale is continuously normalized to the maximum amplitude of the pulse. Color plays a crucial role here in identifying the different components of the amplifier.

Simpler examples in this category merely show a function of a single variable as a curve on the screen; when the movie runs, this curve changes its shape to show the effect of a second variable. In a great many examples of this kind of movie, "movie time" is made to stand for real time in the model (although altered in scale where appropriate). There is no reason in principle why movie time should not represent any arbitrary variable, say a length, while model time takes one of the coordinate axes on the screen. But in practice movie time is not a free parameter; the connection in the viewer's mind with real time is too strong. For example, in the moving-molecule films such as Max's shown on the cover, rotation could imply a polar-coordinate system in which we are shown projections of the solid onto the two-dimensional screen at different values of angle θ. But in practice it becomes, perceptually, simply a rotating molecule, twisting as if suspended on an invisible thread.

From the available examples of time-varying phenomena I have chosen frames from a movie by Frederick D. Tappert of New York University (now at the University of Miami). He is studying the self-focussing of laser beams in nonlinear media, and his film (made at Los Alamos) is remarkable for the way in which information is packed in. On each frame (figure 7) appear both one- and two-dimensional contemporaneous solutions of his equations (intensity curves and spectra in one dimension, contour plots and surface plots in two dimensions). The film has been criticized, I believe unfairly, on the grounds that it is too "busy" and difficult to follow. The complaint only stands if the movie is regarded as a piece of showmanship for nonspecialist audiences. Tappert's is a workmanlike movie that does its job.

We started this article with a couple of colorful and very approachable films that are a pleasure to view simply as art forms. We ended with an example of a black-and-white technical movie that offers nothing to the nonspecialist. Within this wide range the opportunities for further movie making are broad and the potential benefits very great.

References

1. The *Proceedings* of the Boulder conference takes the form of a 40-minute movie, "Computer Movies for Research, 1978," (J. H. Eberly, D. G. Hummer, eds) produced for the National Science Foundation at Lawrence Livermore Laboratory by G. Michael.
2. L. Tilling, Brit. J. Hist. Sci. **8**, 193 (1975).
3. G. H. Gilmer, K. A. Jackson, Current Topics in Material Science **2**, 79 (1977); J. D. Weeks, G. H. Gilmer, in Adv. Chem. Phys. **40** (1979), to be published.
4. R. H. Miller, Astrophys. J. **223**, 122 (1978).
5. T. Valencich, D. L. Bunker, J. Chem. Phys. **61**, 21 (1974).
6. J. C. Goldstein, D. O. Dickman, Los Alamos publication LA-UR-76-1292. □