Monte-Carlo Method Computes Boltzmann Collision Integral

Because of interest in rarefied-gas-flow problems of space flight and upper-atmosphere physics, the method of solving the nonlinear Boltzmann equation has received increasing attention from many researchers. Local, strong departure from thermal equilibrium (as in a shock wave) makes rarefied-gas-flow problems different from continuum problems. The collision integral in the Boltzmann equation is directly related to this departure from equilibrium and must, therefore, be evaluated in thorough studies of rarefied-gas-dynamic phenomena. It is well known that the intractability of this integral blocked attempts to solve the Boltzmann equation and prevented the full use of kinetic theory for nonlinear problems.

The workshop on Monte-Carlo solutions of the Boltzmann equation, held in November at the University of Illinois (Coördinated Science Laboratory), transmitted to scientists interested in kinetic theory and numerical methods the details of the Monte-Carlo method of solving the Boltzmann equation and the results of its application to three nonlinear kinetic-theory problems.

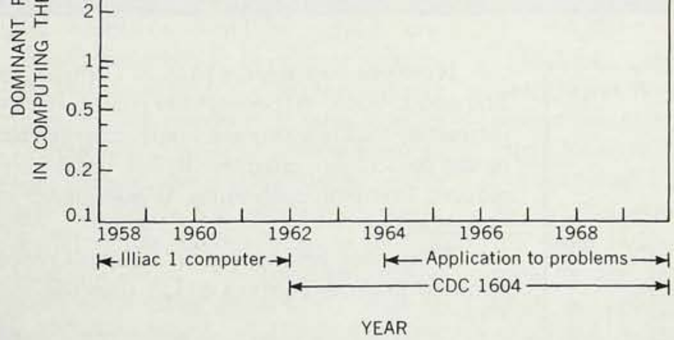
Arnold Nordsieck of the University of Illinois physics department visualized the possibility of developing a Monte-Carlo method for evaluating the collision integral by using a digital computer and devised such a method in 1955. The first computer program was developed in 1958. Since then the method has been refined and extensively tested by the Boltzmann group under the direction of Bruce L. Hicks. The group has applied the method to three kinetic-theory problems, each representing a gas that is far from equilibrium. These problems are the pseudoshock, a translational relaxation problem; the strong shock wave; and heat transfer between two plates at different temperatures.

Improvement in the reliability of the Monte-Carlo computation of the collision integral is illustrated in figure 1. We see that, in the past ten years, there has been a successive reduction in the dominant percent error owing to various modifications and improvements in the Monte-Carlo procedure. The ordinates correspond to a constant computing speed. The length of each solid line indicates the period in which certain dominant error existed in the computation. Not until the beginning of the third period was the dominant error reduced to 2% (owing to two years of careful and systematic study and development of correction procedures). At this time the Boltzmann group started to study the application of Nordsieck's method to kinetic-theory problems. Further reduction of the error, which is expected this year, will expand the range of applicability of the Monte-Carlo method as well as increase the accuracy of the solution of the Boltzmann equation for the problems being studied.

Some computational results are illustrated in figure 2. This shows the lines of constant value of the collision integral (isolines) in the center of a shock wave for Mach number 3. These isolines permit immediate and vivid visualization of the nature of the functions and their changes from one physical or calculational situation to another. The two contour regions shown in this figure characterize the nonequilibrium phenomena in a shock wave. The number on each isoline is the collision integral, I, which is a measure of the local departure from equilibrium. This departure also governs the rate of change of the distribution function at each point $\partial f/\partial x = I/v_x$. The molecules that are in the almost semicircular region near the positive v_x axis decrease rapidly in number while those in the remaining region build up.

Two papers on Nordsieck's method and its application were presented in July 1966 at the Fifth International Symposium on Rarefied Gas Dynamics at Oxford University, and several other papers on Monte-Carlo solutions were given at various APS meetings. These papers provoked much interest because Nordsieck's method was the first and only method of accurately evaluating the Boltzmann collision integral and solving the Boltzmann equation for conditions far from equilibrium. In these papers it was not, however, possible to explain the full details of the Monte-Carlo research work that has extended over a decade.

To make the Monte-Carlo method well known to other researchers and to spread its use outside the University



REDUCTION of dominant percentage error in the collision integral in the period 1958 to the present, with a projection to 1970. Error is now less than 1%. —FIG. 1

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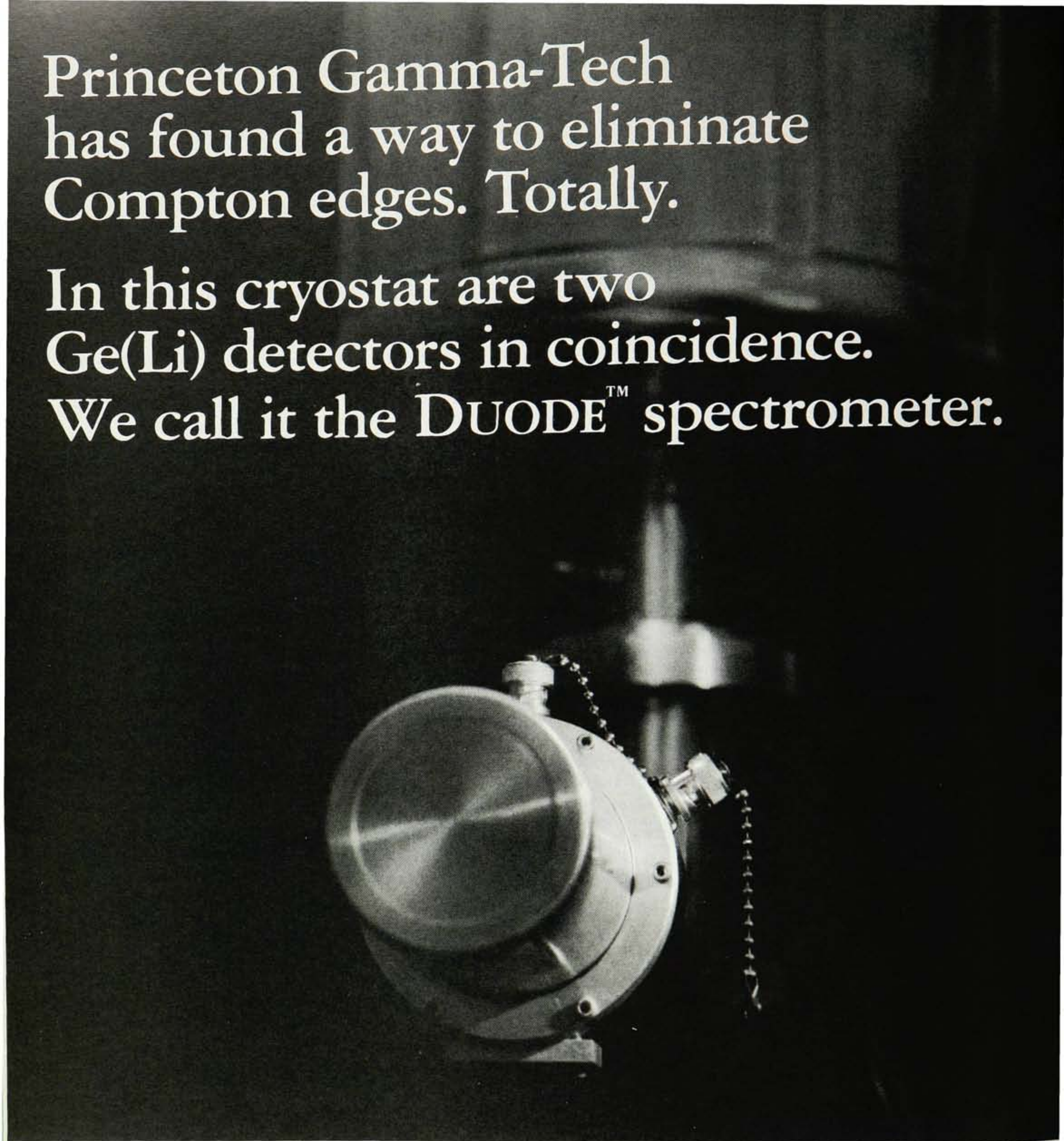

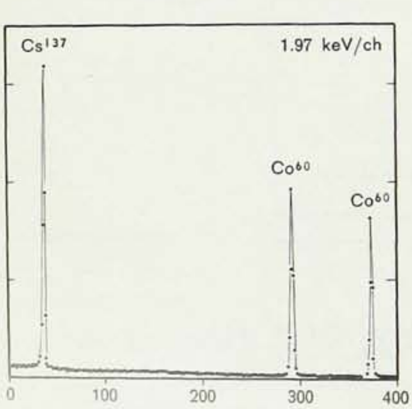

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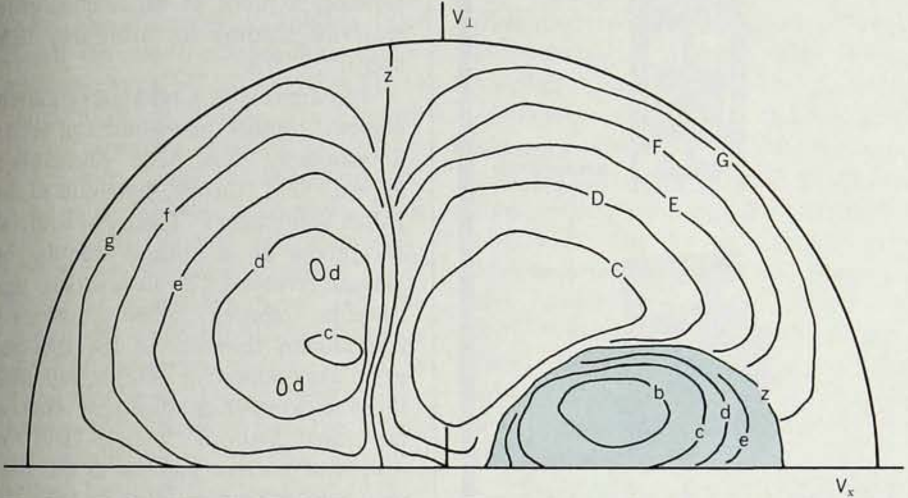
of Illinois, the Boltzmann group organized the workshop on Monte-Carlo solutions of the Boltzmann equation. The first two days of the workshop were devoted to basic considerations in the design of the Monte-Carlo method; the technical problems that have been solved in making the method work properly; the techniques that have led to convergence of iterative solutions of the Boltzmann equation; studies of statistical, quadrature and cutoff errors; and the methods of monitoring the large, relevant volume of computer output.

The last part of the program dealt with new Boltzmann problems and new computers. David Kuch of the department of computer science at the University of Illinois described ILLIAC IV—a very large parallel computer designed in the department and scheduled to operate in 1970. His discussion made it possible to consider in some detail the suitability of such a computer for applying the Monte-Carlo method to more complex problems, such as those involving internal degrees of freedom, mixtures of gases and several independent variables.

Now that more experts in kinetic theory and numerical methods are familiar with the Boltzmann work at the University of Illinois, we hope that the Monte-Carlo results will become more useful in various ways, both to these experts and to other research people interested in nonlinear problems in kinetic theory.



LINES OF CONSTANT VALUE of the collision integral for the center of a Mott-Smith shock wave in a gas of elastic spheres. The region in which molecules decrease in number is in color. A = 0.3, B = 0.1, C = 0.03, D = 0.01, E = 0.003, F = 0.001, G = 0.0003, H = 0.0001, z = 0, b = −0.1, c = −0.03, d = −0.01, e = −0.003. Collision integral measures local departure from equilibrium. —FIG. 2

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The workshop was organized in the Coördinated Science Laboratory at the University of Illinois. The research on rarefied-gas dynamics conducted in the laboratory is supported in part by the Joint Services Electronics Program and in part by the Office of Naval Research.

SHEE-MANG YEN
Coördinated Science Laboratory
University of Illinois

Particle Physicists Look for Dynamics

No new symmetries were proposed, and no new groups emerged to be grappled with, at the fifth Coral Gables conference on symmetry principles at high energy that was held last January at the University of Miami. But there was a sense of satisfaction that at last we are coming to grips with dynamics, the traditional business of physics. Progress towards this goal *via* symmetry, the direction emphasized at the Coral Gables meetings, has seemed to be relatively slow, partly because successes a year later have been taken for granted while failures remain to haunt us. I do not mean to minimize in any way the progress achieved in the meanwhile by the approach that begins with analyticity, unitarity and crossing symmetry of scattering amplitudes, and leads to dispersion relations, bootstrap, Reggeism and perhaps, thus, on to symmetry.

Locklainn O'Raifeartaigh (Institute for Advanced Study, Princeton), in his summary and review of combined space–time interval symmetries, emphasized the point of view that symmetries can lead us to dynamics. He discussed the infinite-component wave functions that were proposed in the early 1930's by Ettore Majorana and revived about a year ago by Yoichiro Nambu. O'Raifeartaigh contended that the last four years' development, involving such diverse approaches as Murray Gell-Mann's relativistic quarks and his current algebra, the $\tilde{U}(12)$ and SL(6,c) groups, the Yukawa bi-local-field theory, as well as many other approaches, all lead inevitably to infinite-component wave equations. Among possible applications, assuming the equations could be solved, one should immediately have mass spectra, electromagnetic form factors, decay rates for strong decays, saturation of the current algebra at infinite momentum with single-particle states, and a way to solve the relativistic quark model. The approach is, therefore, very ambitious and, correspondingly, beset with many difficulties. One of these difficulties has been that a mass spectrum is obtained in which mass values of the states decrease with increasing spin, in contradiction to the observations. More recently it has been possible to prescribe the mass spectrum desired; that is, to introduce it into the problem *a priori*. Obviously, if this is true one loses an important prediction. In addition, there appears to be considerable doubt that acceptable (that is, mathematically stable) solutions of the equations exist corresponding to a particular class of particles, for example mesons alone, so that one may be forced to tackle the truly formidable task of obtaining *all* the particle states in order to have any solution at all. Nevertheless that does not mean that a great deal cannot be learned in the attempt.

Stability criterion. A related, though much simpler, case was discussed by Arthur Wightman (Princeton) from the axiomatic viewpoint. He exhibited a criterion for the stability of the acceptable solutions valid for finite-component wave equations such as the Rarita–Schwinger equations of spin-3/2 particles. These equations usually have unphysical solutions in addition to the desired physical ones, and these solutions are likely to appear in final states of a