The Monte Carlo Method

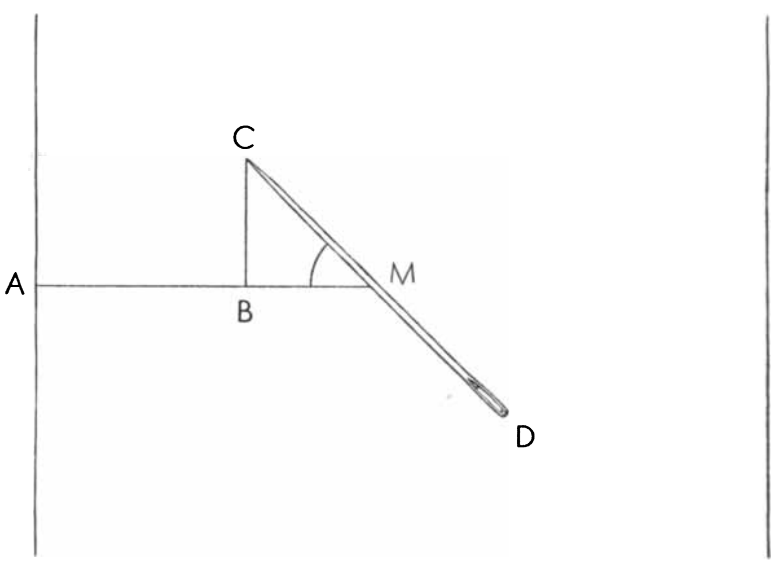
It is used to predict the outcome of a series of events, each of which has its own probability. Here it is outlined in terms of neutrons, needles, roulette wheels and furniture factories

by Daniel D. McCracken

During World War II physicists at the Los Alamos Scientific Laboratory came to a knotty problem on the behavior of neutrons. How far would neutrons travel through various materials? The question had a vital bearing on shielding and other practical considerations. But it was an extremely complicated one to answer. To explore it by experimental trial and error would have been expensive, time-consuming and hazardous. On the other hand, the problem seemed beyond the reach of theoretical calculations. The physicists had most of the necessary basic data: they knew the average distance a neutron of a given speed would travel in a given substance before it collided with an atomic nucleus, what the probabilities were that the neutron would bounce off instead of being absorbed by the nucleus, how much energy the neutron was likely to lose after a given collision, and so on. However, to sum all this up in a practicable formula for predicting the outcome of a whole sequence of such events was impossible.

At this crisis the mathematicians John von Neumann and Stanislas Ulam cut the Gordian knot with a remarkably simple stroke. They suggested a solution which in effect amounts to submitting the problem to a roulette wheel. Step by step the probabilities of the separate events are merged into a composite picture which gives an approximate but workable answer to the problem.

The mathematical technique von Neumann and Ulam applied had been known for many years. When it was revived for the secret work at Los Alamos, von Neumann gave it the code name "Monte Carlo." The Monte Carlo method was so successful on neutron diffusion problems that its popularity later spread. It is now being used in various fields, notably in operations research.



NEEDLE PROBLEM is illustrated by a needle lying on a piece of paper ruled with parallel lines. The length of the needle is two inches; the distance between the lines, four inches. If the needle is thrown on the paper at random, how often will it land on one of the lines?

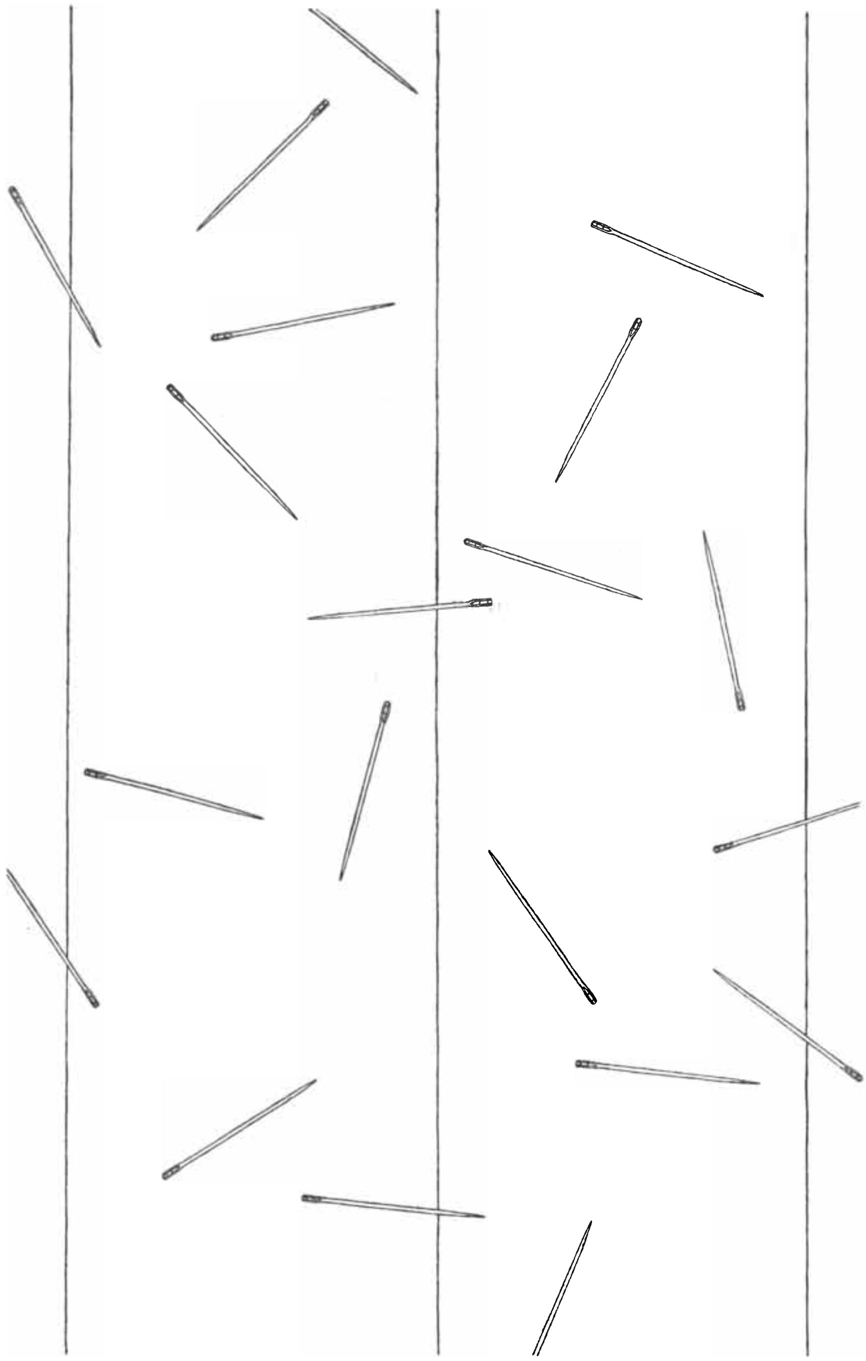
To illustrate the method let us start with the simple, classic Buffon needle problem. You get a short needle, draw on a sheet of paper several parallel lines spaced precisely twice the length of the needle apart, and then toss the needle onto the paper again and again in a random fashion. How often will the needle land on a line? The mathematicians say that the ratio of hits to trials should be 1 to 3.1416. That is, dividing the number of hits into the number of throws, you should come out with the number 3.1416 (pi) if you continue the trials long enough (and throw the needle truly at random, without trying either to hit or to miss the lines).

I tried the experiment, with the following results. In the first 10 throws, the needle landed on a line four times. In the language of the statistician, there were four "successes" in 10 trials. The quotient is 2.5, which one must admit is not very close to 3.1416. In 100 trials there were 28 hits for an estimate of 3.57, also not good, but better. After 1,000 trials there were 333 hits for an estimate of 3, and my arm was tired.

This was hardly good enough to quit on, but the improvement with increasing numbers was not rapid, so it did not seem practicable to go on by hand. The fact is that the accuracy of a Monte Carlo approximation improves only as the square of the number of trials: to double the expected accuracy of the answer, you must quadruple the number of trials. I decided to make a calculating machine do the work, and I translated the problem to a medium-sized electronic calculator.

It is no difficult matter to make a calculating machine carry out operations which simulate the results of dropping a needle on ruled paper. Consider the diagram on the opposite page. To describe the situation to the machine we must decide on a way of specifying the position of the needle relative to the nearest line. It does not matter on which side of this line the needle lies; nothing is changed if we turn the paper around. We can see that the distance from the midpoint of the needle to the nearest line (MA) is specified by a number between zero and two inches. The only other information needed to specify the position of the needle completely is the angle it makes with the perpendicular (MA) to the line. The angle is somewhere between zero and 90 degrees (not 180 degrees, because we are concerned only with the closer end of the needle). Given these two quantities, the machine can easily decide whether the needle touches a line; all it needs to do is to compute the distance MB (the cosine of the angle) and note whether it is less or greater than the distance MA—in the machine's terms, whether the difference is positive or negative.

Now to find out by experiment in what proportion of the trials a needle dropped at random would touch the line, we would like to test all possible positions in which the needle might land. To do this we would have to consider all possible combinations of distances and angles—essentially the method of the integral calculus. Obviously we are not going to tackle this infinite task. But in place of attempting a systematic exploration of all positions, we can take a random sample of them, and this should give us a reasonably accurate approximation of the correct answer, as a sampling poll may do.



ACTUAL EXPERIMENT on the needle problem was tried by artist Eric Mose. Each needle represents a toss and shows the position in which the needle landed with respect to the lines. In a sufficiently large number of trials, the ratio of hits to trials will be 1 to 3.1416 or pi.

How shall we select the random sample? This is where the Monte Carlo method comes in. Suppose we built a roulette wheel with 20 compartments, representing 20 different distances from the line (up to two inches) for the needle midpoint. A spin of the wheel would select the distance for us in a random manner, and over many trials each of the 20 distances would be selected about the same number of times. With a similar wheel we would pick the angle each time in the same random fashion. Then a series of spins of the two wheels would give us a random set of positions, just as if we had actually dropped a needle at random on ruled paper.

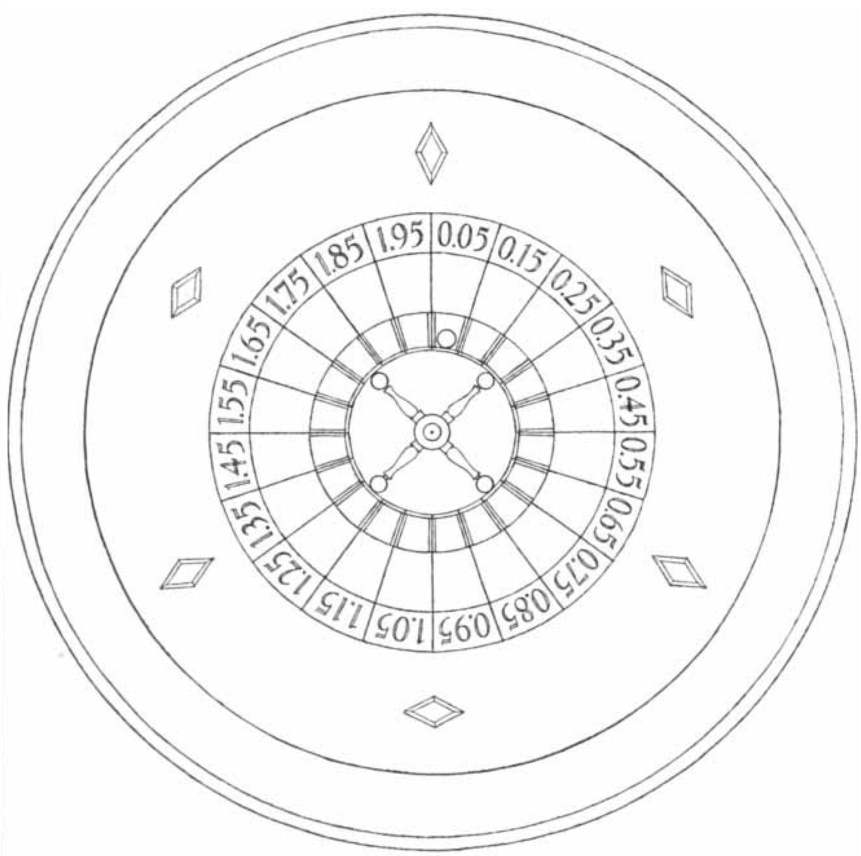
Of course the wheel-spinning method would be more cumbersome than dropping the needle, but there are ways of doing about the same thing with numbers and a calculating machine. First we get up two lists of numbers: one for distances in the range between zero and two inches, the other for angles in the range between zero and 90 degrees. The numbers are chosen at random to cover the whole range in each case without favoring any part of the range; we can take them from some list of numbers already checked for randomness or we can make our own list from, say, a table of logarithms, taking the numbers' last three digits. Then we put the calculator to work computing whether various combinations of the distance and angle numbers place the needle on a line or not (*i.e.*, whether the difference between MB and MA is positive or negative). Repeating the operation many, many times, we can get as close to precision as we like; statistical principles tell us the degree of precision we can expect from a given number of trials.

The moderately fast computer I had available when I made the experiment was able to perform 100 "trials" per minute. In about an hour the machine ran through 6,000 trials, and there were 1,925 "hits." In other words, the estimate of pi was 3.12, which is as good as can be expected for 6,000 trials.

Even this simple case required a rapid computer. Most applications of the Monte Carlo method of course are much more complex. However, the present high-speed computers make them feasible: there are machines which can perform 5,000 trials per minute on the Buffon needle problem.

Let us see now how the method works on a simple problem in neutron diffusion. Suppose we want to know what percentage of the neutrons in a given beam would get through a tank of water of a given size without being absorbed or losing most of their speed. No formula could describe precisely the fate of all the neutrons. The Monte Carlo approach consists in pretending to trace the "life histories" of a large sample of neutrons in the beam. We imagine the neutrons wandering about in the water and colliding occasionally with a hydrogen or oxygen nucleus—remember that to a neutron water looks like vast open spaces dotted here and there with tiny nuclei. We shall follow our neutrons one by one through their adventures.

We know how far a neutron travels, on the average, before it encounters a nucleus, the relative probability that this encounter will be with oxygen or with hydrogen, the relative chances that the neutron will be absorbed by the nucleus or bounce off, and certain other necessary information. Let us, then, take a specific neutron and follow its life history. It is a slow-moving neutron, and its first incident is a collision with a hydrogen nucleus. We know (from experiments) that the chances are 100 to one the neutron will bounce off from such a



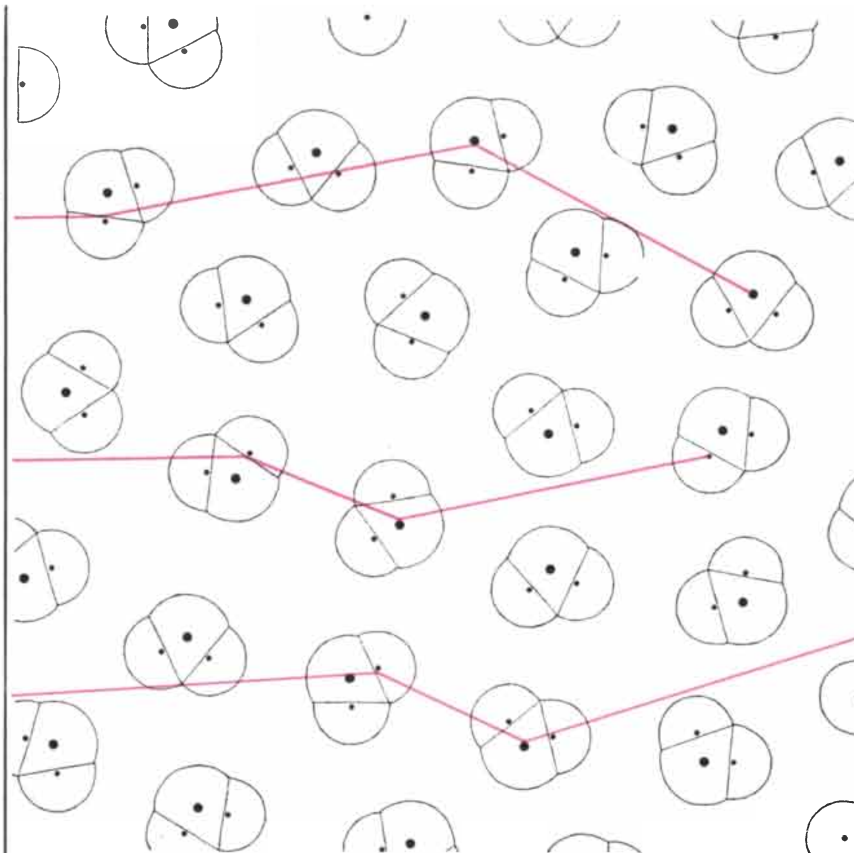
ROULETTE WHEEL especially designed for the needle problem depicted on the preceding two pages illustrates a basic feature of the Monte Carlo method. Each compartment of the wheel represents one of 20 distances between zero and two inches, the length of the needle.

collision. To decide what it will do in this instance, we figuratively spin a roulette wheel with 100 equal compartments marked "bounced off" and one marked "absorbed." If the wheel says "absorbed," that is the end of the neutron's history. If it says "bounced off," we perhaps spin another appropriately marked wheel to decide what the neutron's new direction is and how much energy it lost. Then we must spin another wheel to decide how far it travels to the next collision and whether that collision is with oxygen or hydrogen. Thus we follow the neutron until it is absorbed, loses so much energy that it is no longer of interest or gets out of the tank. We go on to accumulate a large number of such histories and obtain a more or less precise figure for the percentage of neutrons that would escape from the tank. The degree of precision depends on the number of trials.

In practice, of course, we do not use roulette wheels but random numbers, as in the previous example. I have omitted much of the detail of the calculation for the sake of simplicity and clarity. In one very simple problem on which I assisted, an electronic calculator labored for three hours to trace the life histories of 10,000 neutrons through 1.5 million collisions. I would have had to sit at a desk calculator for some years to accomplish the same results.

As a third illustration of the Monte Carlo method, let us take a simple problem in operations research. Imagine a woodworking shop consisting of a lathe, a drill press and a saw, with three men to operate the machines. The shop makes one model of chair and one model of table. The question is: How should the work of the shop be scheduled to yield the greatest production, considering a number of variable conditions affecting output?

Certain basic information must be gathered before any calculation can begin. How long does it take on each machine to do the necessary work on each piece of wood? How much does the time needed for each job fluctuate because of fatigue, boredom or other personal factors? How frequently do the machines break down? After the data are gathered, a way is devised to make the computer simulate the operation of the shop under specified conditions of scheduling. We will not go into the details here; perhaps enough has been presented in the other examples to give an indication of what has to be done. The computation is properly classified as Monte Carlo because it is necessary to spin a roulette



NEUTRONS wander through water in a series of events, each with a known probability. Here the microscopic structure of water is depicted in highly idealized form as consisting of simple molecules of H_2O. The larger sphere in each molecule is oxygen; the two smaller spheres are hydrogen. The neutrons (*colored lines*) may be absorbed by either an oxygen or a hydrogen nucleus or may bounce off from the collision. Some may escape from the water.

wheel, or the equivalent, to pick samples from the known distributions. For example, we may know that a certain job may take anywhere from 12 to 16 minutes, and we have noted the percentages of the cases in which it is performed in 12, 13, 14, 15 and 16 minutes respectively. Which time shall we use for a particular case as we follow the course of a day's work in the shop? The question must be decided by random sampling of the type I have described.

With the Monte Carlo method high-speed computers can answer such questions as these: How should the schedule be changed to accommodate a market change demanding twice as many chairs as tables? How much could the shop produce, and at what cost, if one man should be absent for two days? How much would the total output be increased if one man should increase his work rate 20 per cent? Under a given schedule of work flow, what percentage of the time are the men idle because the work is piled up behind a bottleneck machine? If money values can be assigned to idle time, loss of orders due to low production and so on, dollars-and-cents answers can be given to problems of this kind in business operation.

The Monte Carlo method, in general, is used to solve problems which depend in some important way upon probability—problems where physical experimentation is impracticable and the creation of an exact formula is impossible. Often the process we wish to study consists of a long sequence of steps, each of which involves probability, as for instance the travels of the neutron through matter. We can write mathematical formulas for the probabilities at each collision, but we are often not able to write anything useful for the probabilities for the entire sequence.

Essentially the Monte Carlo method goes back to probability theory, which was developed from studies of gambling games. But it takes the opposite approach. The mathematicians who originated the probability theory derived their equations from theoretical questions based on the phenomenon of chance; the Monte Carlo method tries

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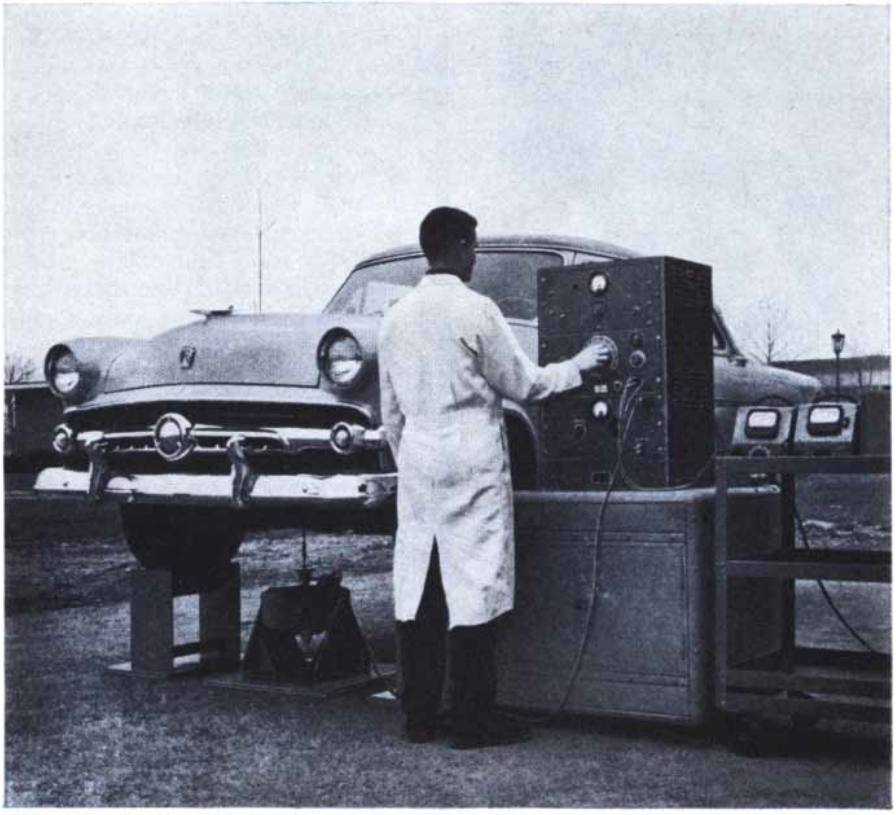

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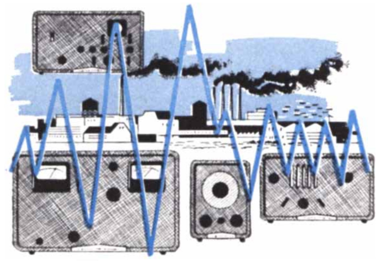

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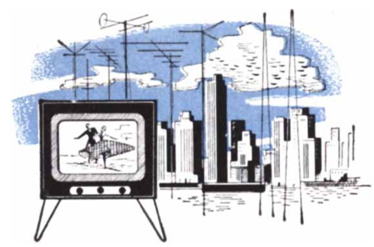

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to use probability to find an answer to a physical question often having no relation to probability.

In the neutron problem, for example, the investigator's thinking might have been along these lines: "I have a physical situation which I wish to study. I don't think I'll even try to find an equation representing the entire problem. Even if I could find one, which is very doubtful, I probably wouldn't be able to get much useful information out of it. I'll just see if I can't find a game of chance which will give an answer to my questions, without ever going through the step of deriving an equation." In some other situations the investigator would reason: "The physical situation I am interested in has resulted in an equation which is very difficult to solve. I cannot possibly solve it in any reasonable length of time by usual methods. I wonder if I could devise some statistical method which would approximate the answer to my problem."

Much work remains to be done on the method. One is always faced with the unhappy choice of either inaccurate results or very large amounts of calculation. A problem which demands 100 million trials of some "experiment" is still impracticable, even on the fastest present computers. Another difficulty is that it is seldom possible to extend the results of a Monte Carlo calculation to another set of conditions. For instance, after we have solved the problem of the passage of neutrons through ordinary water, we have to start all over again to find out how they will behave in heavy water. Nevertheless, in spite of its various limitations the Monte Carlo method is able to give at least approximate answers to many questions where other mathematical techniques fail.

Many mathematicians are working to improve the method, especially to reduce the computation required and to determine exactly how much reliability can be attributed to its results in various types of problems. Up to now the technique has been used mainly on problems of nuclear physics, such as the diffusion of neutrons, the absorption of gamma rays, atomic pile shielding and the like. In the author's opinion, one of the most promising applications of the method is in operations research. It could be useful not only on production problems such as the one described here but also in telephone operation, traffic control, department-store inventory control and so on. Some of these possibilities are already being investigated. It is safe to say that we shall hear more from Monte Carlo in the next few years.

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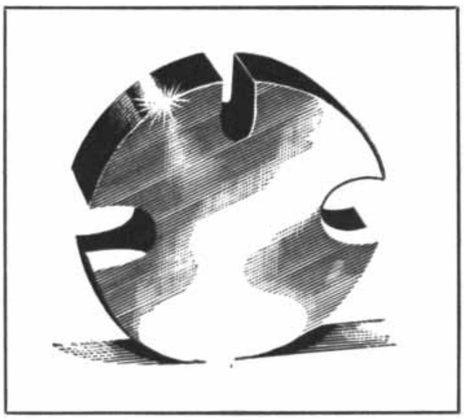

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