METHODS IN COMPUTATIONAL PHYSICS

Advances in Research and Applications

Edited by

Berni Alder

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Volume 1

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Volume 1

Statistical Physics

1963

ACADEMIC PRESS

NEW YORK AND LONDON

ACADEMIC PRESS INC.
111 Fifth Avenue, New York 3, New York

United Kingdom Edition published by
ACADEMIC PRESS INC. (LONDON) LTD.
Berkeley Square House, London W.1

LIBRARY OF CONGRESS CATALOG CARD NUMBER: 63-18406

PRINTED IN THE UNITED STATES OF AMERICA

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Preface

The computer has become the laboratory tool of the theoretical scientist. With it he hopes to learn new things which were previously inaccessible, in very much the same way as an experimentalist employs a piece of equipment. This hope depends to a large extent on the development of new methods designed specifically for the computer. The major aim of this series of books is to collect these techniques which were developed in the solution of physical problems.

The theoretical advances which can be made by this new tool appears to be enormous and in many different areas of science. In chemistry and physics, for example, many of the theoretical problems that are faced are mathematical in nature, the physical laws being well established. If, for example, the Schroedinger equation could be solved for more than two particles, molecular chemistry would become quantitative. To solve such problems, the first tendency is to transfer the well established techniques from the desk calculator to the high speed computer. In this way much can be learned by obtaining more accurate and extensive solutions. Alternatively, however, new methods should be thought about which are made practicable only by having access to a machine able to perform arithmetic at high speeds. It is the development of these new methods which we would particularly like to encourage in this series.

It is for this reason that our first volume covers mainly various aspects of the Monte Carlo method. This method is only suited for a high speed computer and permits the accurate numerical solution of many problems which are only approximately soluble by analytical techniques. In fact, the method was used in one of the first applications of computers, namely, the scattering of neutrons by a wall. Chapters *2* through *5* in this volume give the more recent applications and methods to the scattering of various particles. Chapter *1*, by way of contrast gives a competing method for solving the neutron transport problem. The last three chapters are concerned with application of the Monte Carlo method to problems in statistical mechanics. There are many more applications involving variations on the Monte Carlo method and it is hoped that another volume in the future will be devoted to these.

In the effort to make computers a more useful tool to the physical scientist, we feel it desirable to complement the scientific journals by reversing the emphasis between computational detail and physical results. This is because

scientific journals, owing to space limitation, discourage detailed exposition of numerical techniques, even though these techniques are time consuming to develop, and frequently crucial to the solution of the problem. The policy has thus been established that a typical article would contain a statement of the physical situation in which the problem arose, previous analytical attempts, if any, for its solution, numerical techniques which were used (even those that were unsuccessful), a flow diagram if the problem is of general interest, the advantage and limitation of the method, the memory requirements of the program, the accuracy and convergence of the method and how they were ascertained, description of the numerical results, and so on.

It is hoped that the detailed description of techniques will lead to the development of even better techniques. By pooling experiences it should also lead to more efficient use of computers. Furthermore, we hope to expose those as yet not familiar with computers to the power of these tools. The results also ought to impress the skeptics who like to employ only analytical methods. Numerical solutions are never as general and as compact as analytical solutions. Nevertheless, the two methods complement each other in that a numerical solution tabulates a function in terms of which other problems can then be analytically expressed and, conversely, much analysis has to be done before a new numerical method is developed.

Much progress and activity can be expected in this field now that large computers have become generally available. In the next volume we hope to collect recent numerical advances in the field of quantum mechanics. The subsequent volume will be devoted to the field of hydrodynamics.

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April 1963

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The Numerical Theory of Neutron Transport

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I. Introduction

A. General Principles

The basic relations in neutron transport theory derive from simple statements regarding continuity of neutron flow and numerical balance of the number of particles involved. Neutrons moving into [leaving] a region D of space are also, at the instant they cross the boundaries of D, leaving [moving into] adjoining regions. The neutron properties: number, direction of motion, and velocity are not altered in the process. Continuous flow implies, then, the absence of interference at boundaries.

Statements of balance, for D during a time Δt, for example, equate change in neutron population to gains minus losses. Such statements are usually made for a set of neutron beams, each beam having a fixed direction and velocity. Neutrons flowing into D and those released by sources in D constitute the gains. Neutrons flowing out of D and those removed by the material in D make up the losses. By removals we really mean events leading to beam attenuation, that is, collisions between neutrons and the nuclei of the material. There are no collisions in D if D is in a vacuum. The rectilinear motion of neutrons between collisions is referred to as streaming.

It is assumed that very large numbers of neutrons are involved so that only their average behavior is of concern, and not the departures from that average. Also, in general, one can neglect neutron-neutron interactions entirely, which means that the neutrons flowing through a region D need not be counted as part of the material in D. This has the very important consequence that the equations for neutron transport are linear and thus much more amenable to solution than are the nonlinear equations found for particle movement in gases or plasmas.

Sources may be of the surface type, neutrons per unit area per unit time, or of the volume type, neutrons per unit volume per unit time. Familiar surface sources are sources incident on the outer boundaries of systems (configurations, arrangements of materials) under study. In numerical treatment, surface sources are placed in the immediate vicinity of boundaries rather than right on them. This is in order to make it clear to what region they belong. Commonly occurring volume sources are the reemission sources, for example, the neutrons which after collision emerge scattered. Collisions are permitted to change the properties of the neutrons, that is, their number, direction, and velocity. A collision without change is not generally counted as a net collision. In combination, collision and volume source terms provide the mechanism for transferring neutrons between the various neutron beams of fixed direction and velocity. Sources external to a system, in time or space, are usually labeled initial values, or boundary values, respectively.

It is further assumed that the materials in the system are specified with respect to macroscopic properties, such as location, density, and isotopic composition, and with respect to microscopic character including interactions with neutrons, such as capture cross section, scattering cross section, and fission cross section. The cross sections depend on the velocity of the incident neutron as well as on the isotope with which the neutron interacts. The cross-section data are often given as functions of energy or lethargy rather than velocity, and include data about the released neutrons, that is, data about number (zero in the event of

capture), velocity, and deflection cosine. Together, this information is used to calculate transfer cross sections which after multiplication by a density factor become transfer probabilities (macroscopic cross sections) in terms of events, such as captures, per unit length of neutron travel.

To supply a program of calculation with transfer cross sections is a considerable undertaking in view of the various difficulties with the basic data and the rather elaborate processing required. The cross sections often exhibit a complex resonance structure in energy and also correlation between energy and deflection angle in scattering. The precision of the experimental data is varying and seldom entirely adequate. In some areas data are entirely lacking.

The basic problem in the processing of cross sections is that of reducing continuous and often complicated sets of data to relatively small sets, without losing significantly in realism in the description of materials and their interactions with neutrons. The averaging rules, which one sets up and follows, inevitably make broad assumptions about the applications one has in mind, in particular about the neutron spectrum in energy which one expects within velocity groups. With sets of transfer cross sections are associated, therefore, statements specifying under what general conditions they may be applicable.

The cross-section compilations for the elements in the periodic table are updated from time to time as new or better data accumulate (Hughes and Schwartz, 1958; Argonne National Laboratory, 1958). An increasing number of cross sections are calculated from nuclear models. Also, the techniques for preparing the basic data for use in computation are advancing. Nevertheless, the cross-section problem in transport calculations remains a serious one. It should always be given careful attention.

Finally, it is assumed here that the materials in the configuration are at rest and have properties constant in time, or rather, that changes in these areas, if any, are relatively slow so that the combined problem, neutron transport with material changes, can be replaced by two problems interleaved in time: neutron transport for a short time with fixed material, change of material as indicated by motions, collisions, etc., during that time; then neutron transport for the next time cycle, another change of material, and so forth.

B. Comments on Development of Theory

Transport theory has developed quite swiftly during the last two decades. Much of the stimulus for the development came from problems connected with the design and operation of nuclear reactors. Methods

from mathematical analysis were the main tools during the early period. Important basic results were obtained then by S. Chandrasekhar, in connection with the study of radiation flow in stellar atmospheres, and by G. Placzek and co-workers (among them B. Davison) in the Montreal group, mainly concerned with neutron problems. Many of the developments occurred during the time of World War II, in widely separated places at about the same time.

The general objective in transport theory is the determination of neutron flux, i.e., neutron flow per unit time, across unit area, from a difference or differential equation and as a function of time, position in space, direction in space, and neutron energy.

The analytical techniques first used did not really suffice—the problems were usually too complex—but helped along by simplifying assumptions, by ingenuity and innovation, and by judicious choice of calculations, the techniques proved quite effective in a variety of problems and over many years. They created, in fact, a large number of main topics within transport theory: Simple diffusion theory, Spherical harmonics, Age theory, Serber-Wilson technique, Integral theory, and several others. As the problems increased in complexity the analytical approach became increasingly strained. But then—and to some extent as a consequence—the high-speed computer emerged on the scene. With this revolution in computation, the emphasis shifted to numerical methods, first to methods effective within the separate topics of the theory, and then, somewhat later, to methods attacking the problem of transport directly, starting from first principles. Numerical methods are now clearly the most versatile tools in the field, provided that means of rapid computation are fairly accessible.

It is quite clear that many results in transport theory related to the existence of solutions, asymptotic behavior, series expansions, etc., and obtained by analytical means, cannot readily be deduced from difference equations or by the use of difference methods. For this and other obvious reasons, analytical and semianalytical methods will continue to play important, although somewhat changed roles in the theory. They remain important in the numerical context to help answer, for example, these basic questions: How do numerical results depend on the fineness of resolution specified for the variables? How do the various numerical methods compare? Analytical and numerical methods, separately, provide some, usually not very precise answers. Results from physical experiments, on the other hand, such as critical assemblies, are often compared as follows: experimental results to theoretical results to cross-section data used. This comparison is most often used to modify the cross sections until experiment and theoretical model come to

reasonable agreement, a use which is quite sensible, generally, but precludes help with the questions just posed. Comparisons between numerical and analytical results for simple problems, where both sets of results can be obtained, remain, therefore, among the better means for gaining information about resolution and for judging numerical methods. Chandrasekhar (1960), Davison (1957) and Case *et al.* (1953), to mention only a few of the analysts, provide numerous opportunities along these lines.

A few basic numerical techniques and most of the methods for simplifying problems and theoretical description were introduced in the early period. The discrete method for handling neutron flux as a function of direction was introduced then. This method was first suggested by G. Wick but was mainly developed by S. Chandrasekhar (see Davison, 1957, pp. 174-182). Variations on it appeared later, an important one is from J. Yvon (see Davison, 1957, pp. 171-173). Early efforts in simplification produced the special topics within transport theory as mentioned previously and also the first methods for eliminating variables, processing cross sections, treating scattering laws, etc.

The main object of this article is to give the most general formulation possible at this time of a numerical theory of neutron transport. From this is derived a general method for solving neutron transport problems numerically, a method around which particular procedures, the topics of numerical transport theory, may group or develop. The basic difference equation of the theory will be derived directly from the principles and assumptions stated at the beginning.

Since the discrete representation of direction remains, the general formulation and method may be regarded as a generalization of the Wick-Chandrasekhar method. It is usually called the discrete S_n method or simply S_n for convenience and in reference to the first formulation which made the generalization possible. An effort has been made to include here the main information needed for the planning and flow diagramming of S_n calculations and codes, and also, either directly or indirectly through the references given, some guidance to what else is required in actual calculations.

II. Coordinate Systems

A. General Description

The later discussion of difference equations will be made in relation to three familiar and basic space symmetries, rectangular, cylindrical, and spherical. The left-side diagrams of Fig. 1 illustrate the coordinate

systems corresponding to these symmetries. They name the variables of position ($\mathbf{r}$) and direction (Ω), specify the components of the former, and relate these, in the cylindrical and spherical cases, to the rectangular coordinates x, y, and z. Shown also, in each left-side diagram, is a sample neutron path starting at position $\mathbf{r}$ (at point P) and extending some distance (Δs) in the direction Ω.

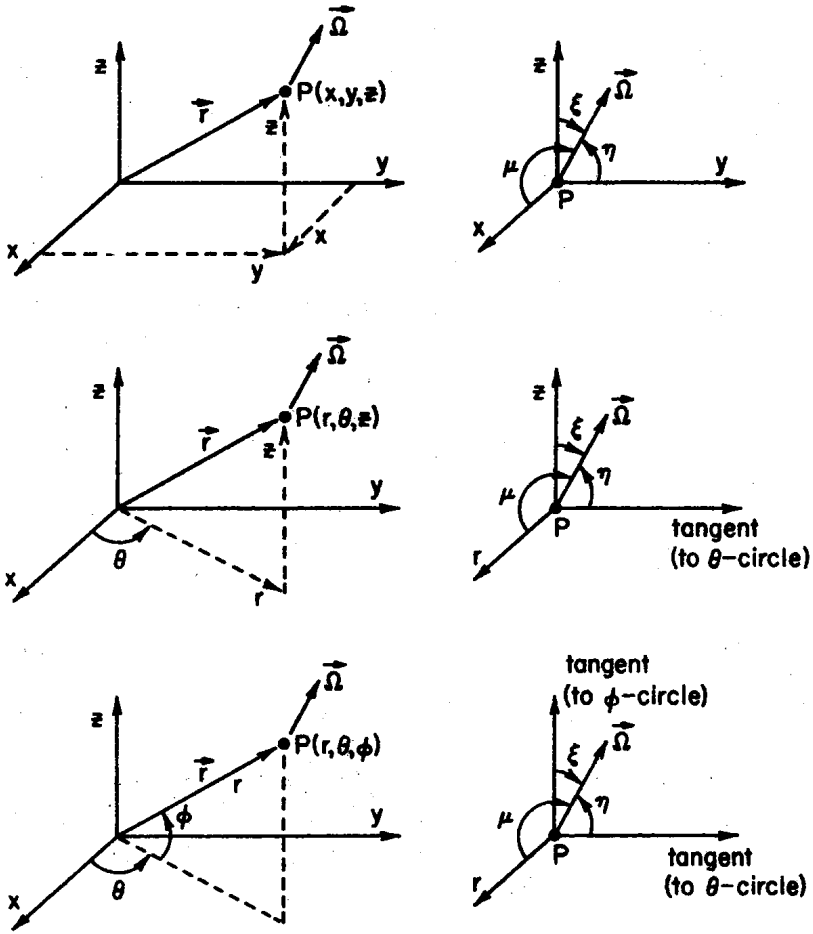

FIG. 1. Coordinate systems; fixed and local frames of reference for rectangular, cylindrical, and spherical symmetries. (Symbols with arrows correspond to boldface symbols in text, and μ, η, and ξ denote cosines.)

In the diagram to the right, again referring to Fig. 1, the components μ, η, and ξ of the unit vector Ω are shown. These are measured with respect to a local frame of reference with origin at P, thereby forming a coordinate triplet for specifying direction. The local reference system

is lined up with the intersecting tangents touching the space coordinate lines, i.e., the grid lines passing through P. It is clearly a rectangular system since the basic geometries we are dealing with are orthogonal. The components of Ω obey, therefore, the relation $\mu^2 + \eta^2 + \xi^2 = 1$. One usually selects one of the components, say μ, as one of the independent variables, and writes the others, η and ξ, in terms of ω, a second one, as follows: $\eta^2 = (1 - \mu^2) \sin^2 \omega$ and $\xi^2 = (1 - \mu^2) \cos^2 \omega$.

The local frame of reference is here regarded as a moving one, attached to the neutron beam and moving with it along a straight line path. Since this frame is also tied to a space-coordinate system, it may change in orientation as it moves, and generally does this in cylindrical and spherical systems where the space coordinates are curvilinear. Neutrons in the process of streaming must therefore be permitted to change direction coordinates. This is beam attenuation quite apart from that provided by the mechanism of collision discussed earlier. The process will be called angular redistribution. It shifts neutrons in direction cosine, for descriptive purposes really, without affecting their number, basic direction, or velocity. It is the expression of continuity of flow unaffected by changes of variable.

Directions may be depicted as points on the surface of a unit sphere. In what follows it may be useful to refer to Fig. 2, which shows octants of unit spheres, and to Fig. 4, which shows the upper front quadrant of one, in perspective. In rectangular coordinate systems no change of direction cosines is possible during streaming. In cylindrical systems, neutron movement causes higher values of μ always with η first increasing while μ remains negative and then decreasing; ξ is uneffected. In spherical systems of full symmetry, i.e., in systems without θ and φ variation, the shift is also toward higher μ. In the general case, however, this pattern is combined with another one: a shift toward smaller values of ω if φ is positive, toward higher values if φ is negative.

There are some special points and lines (great circles) on the unit sphere. In the cylindrical case there is no angular redistribution along the line $\eta = 0$ and none into or out of directions having $\eta = 0$. In the spherical case there is no flow into or out of the directions $\mu = \pm 1$ and no flow into or out of other directions with $\eta = 0$ except by redistribution along the line $\eta = 0$. The neutron flux can readily be calculated for these special directions, a fact that will be made use of later.

B. Mesh Systems in Time and Space

In numerical treatment, discrete variables take the place of continuous ones and vary over domains that are finite sequences rather than inter-

vals. Thus the time variable t in our case is assumed to take on the values t_s, where $s = 0, 1, 2, \ldots$, the elements of the sequence $\{t_s\}$, with steps $\Delta t_s = t_s - t_{s-1}$, where $s = 1, 2, 3, \cdots$. Similarly, the space variable x is assumed to range over x_i, where $i = 0, 1, 2, \ldots$, the elements of $\{x_i\}$, with intervals Δx_i, etc. We now adopt the following conventions. Time is to be represented by t and the subscript s, and position by the coordinate triplets (x, y, z), (r, θ, z), or (r, θ, φ), as the case may be, as well as by subscript triplets (i, j, k), with one-to-one correspondence between elements. Thus, for example, we shall use the terms (r, z) geometry and (i, k) cylindrical geometry interchangeably.

Many factors enter into the choice of geometry and the selection of time and space points. The geometry is most often selected on the basis of the dominating form of the surfaces which define the configuration. Thus, for a right circular cylinder, inside a similar figure and sharing its axis, with no other forms in sight, one obviously chooses cylindrical geometry. Pertinent defining surfaces here are those enclosing the system or separating the materials within it, those carrying surface sources, and those delineating volume sources.

To form a space mesh, that is, to fill all of space with mesh intervals and simultaneously with mesh points, we let the sets $\{x_i\}$, $\{y_j\}$, and $\{z_k\}$, define mutually orthogonal sets of surfaces in space. The mesh interval

TABLE I

AREA AND VOLUME ELEMENTS FOR MESH CELLS IN RECTANGULAR, CYLINDRICAL, AND SPHERICAL COORDINATE SYSTEMS.

Geometry and variables	Area elements A	B	C	Volume element
Rectangular				
x	1	⋯	⋯	Δx_i
x, y	Δy_j	Δx_i	⋯	$\Delta x_i \Delta y_j$
x, y, z	$\Delta y_j \Delta z_k$	$\Delta x_i \Delta z_k$	$\Delta x_i \Delta y_j$	$\Delta x_i \Delta y_j \Delta z_k$
Cylindrical	$C_i = (r_{i+1}^2 - r_i^2)/2$			
r	$2\pi r_i$	⋯	⋯	$2\pi C_i$
r, θ	$r_i \Delta\theta_j$	Δr_i	⋯	$C_i \Delta\theta_j$
r, z	$2\pi r_i \Delta z_k$	⋯	$2\pi C_i$	$2\pi C_i \Delta z_k$
r, θ, z	$r_i \Delta\theta_j \Delta z_k$	$\Delta r_i \Delta z_k$	$r_i \Delta r_i \Delta\theta_j$	$C_i \Delta\theta_j \Delta z_k$
Spherical	$S_i = (r_{i+1}^3 - r_i^3)/3$,	$S_k = (\sin\varphi_{k+1} - \sin\varphi_k)$		
r	$4\pi r_i^2$	⋯	⋯	$4\pi S_i$
r, φ	$2\pi r_i^2 S_k$	⋯	$2\pi C_i \cos\varphi_k$	$2\pi S_i S_k$
r, θ, φ	$r_i^2 \Delta\theta_j S_k$	$C_i \Delta\varphi_k$	$C_i \Delta\theta_j \cos\varphi_k$	$S_i \Delta\theta_j S_k$