CHAPTER 9

NUMERICAL METHODS II

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ABSTRACT

Finite difference techniques for solving the Poisson equation and a steady-state advection-diffusion type equation are discussed. These include direct methods, the Jacobi and Gauss-Seidel iteration methods, the successive overrelation method, and the alternating direction implicit method for the Poisson equation. Upwind difference methods are used to solve the steady-state advection-diffusion type equation. The Galerkin method and its modifications are derived as special cases of the method of weighted residuals. The finite element method is derived via the Galerkin formulation. Monte Carlo methods are introduced. A Monte Carlo procedure for solving Laplace's equation with Dirichlet boundary conditions is presented.

9.1 Introduction

The behaviour of a fluid experiencing convection heat transfer is described by a system of partial differential equations expressing the conservation of mass, momentum, and energy. The fundamental equations for two-dimensional incompressible flow of a Newtonian fluid with no

body forces, no dissipation term and constant properties can be expressed in nondimensional form as:

$$\frac{\partial \xi}{\partial t} = - \vec{\nabla} \cdot (\xi \vec{v}) + \frac{1}{Re} \nabla^2 \xi \ , \tag{9.1}$$

$$\nabla^2 \phi = \xi \ , \tag{9.2}$$

$$\frac{\partial T}{\partial t} = - \vec{\nabla} \cdot (T \vec{v}) + \frac{1}{Pe} \nabla^2 T \ , \tag{9.3}$$

where

$$\xi = \text{vorticity} = \frac{\partial v_x}{\partial y} - \frac{\partial v_y}{\partial x} \ ; \tag{9.4}$$

$$\phi = \text{stream function, with } v_x = \frac{\partial \phi}{\partial y} \text{ and } v_y = - \frac{\partial \phi}{\partial x} \ ; \tag{9.5}$$

T = nondimensional temperature;

$\vec{v} = (v_x, v_y)$ = nondimensional velocity vector;

Re = Reynold's No.;

Pe = Peclet No.

In general, the full system of Equations 9.1-9.5 must be solved simultaneously.

In this chapter, some numerical methods for solving the Poisson equation and a steady-state advection-diffusion type equation as shown below are considered.

$$\nabla^2 u = 0 \tag{9.6}$$

and

$$(\vec{w} \cdot \vec{\nabla}) \, u = D \, \nabla^2 u \tag{9.7}$$

where $\vec{w}$ is a vector velocity field, and D is a diffusion coefficient. Solution of these equations are of central importance in the multidimensional modelling of single phase flow and two-phase flow (Chapt. 8)

9.2 Derivation of Finite Difference Equations to Poisson's Equation

Consider the two-dimensional Poisson's equation in a region R, with boundary S,

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = f(x,y), \quad \text{for } (x,y) \text{ in } R \tag{9.8}$$

with the boundary condition

$$u(x,y) = g(x,y), \quad \text{for } (x,y) \text{ on } S \tag{9.9}$$

A rectangular grid on the region R is set up so that every point (i,j) has four neighbours, as shown in Fig. 9.1. A point (i,j) of the grid is classified as an interior point if its four neighbours lie within R, or on S, but not outside S. Those points in R or S, which are not interior points, are classified as boundary points.

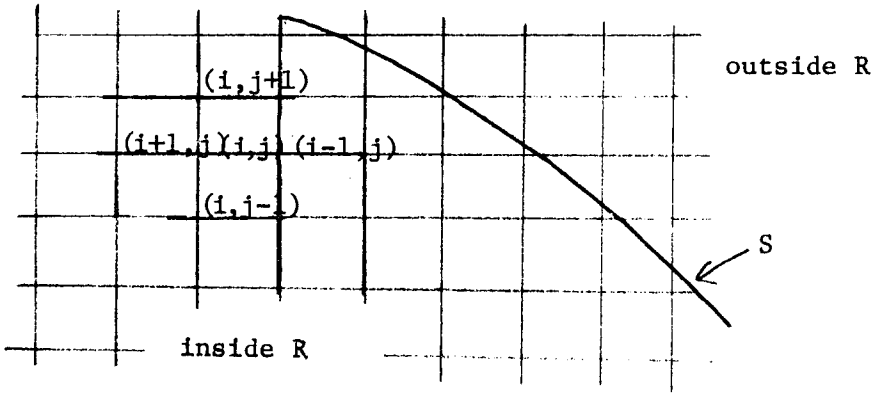

Fig. 9.1 Rectangular Grid

Approximating Eq. 9.8 at each interior point by finite difference,

$$\frac{v_{i+1,j} - 2v_{i,j} + v_{i-1,j}}{\Delta x^2} + \frac{v_{i,j+1} - 2v_{i,j} + v_{i,j-1}}{\Delta y^2} = f_{i,j} \tag{9.10}$$

where $v_{i,j}$ is the approximate solution to $u(x_i,y_j)$ and $f_{i,j} = f(x_i,y_j)$. At each boundary point

$$v_{i,j} = g(x_i,y_j) \tag{9.11}$$

By eliminating from Eq. 9.10 the values of v at the boundary using Eq. 9.11, a system of n linear equations in n values of $v_{i,j}$ for the approximate function at each interior point is obtained. Designating the interior points as v_k, this system of equation can be put in the form

$$A\bar{v} = \bar{b} \tag{9.12}$$

where $\bar{v} = (v_1, v_2, v_3, \ldots, v_n)$ and A is an nxn matrix whose entries are determined by the coefficients of the difference equation, and $\bar{b}$ is determined by the boundary conditions and the known terms in the differential equation. A solution to Eq. 9.12 exists and is unique if and only if A is nonsingular, then

$$\bar{v} = A^{-1}\,\bar{b} \tag{9.13}$$

9.3 Direct Methods

The most elementary methods for solving Eq. 9.12 are Cramer's rule and various forms of Gaussian elimination. Unfortunately, for most systems of interest, the size of the matrix A is so large that the derivation of the inverse by any direct method requires an excessive amount of calculation, in addition to considerations of round-off errors. In recent years, highly efficient direct methods have been developed for some special cases.

9.4 Jacobi and Gauss-Seidel Iteration Method

The Jacobi method, which is a special case of Richardson's method, and the Gauss-Seidel method, also known as Liebman's method, are iterative methods. Basically, each method involves transferring all the off-diagonal terms of Eq. 9.12 to the right hand side, so that the i^{th} equation leads to

$$v_i = (b_i - \sum_{\substack{j=1 \\ j\neq i}}^{n} a_{ij}\, v_j)/a_{ii} \qquad (9.14)$$

By starting with an initial guess of v_j on the right hand side, new approximate values of v_i can be computed from Eq. 9.14. This procedure is repeated until the computed values show little change. It can be shown that for the finite difference equations from Eq. 9.8 and 9.9, the above iterative method is always convergent. The final solution is independent of the choice of starting values, although a poor initial guess will require more iterations for convergence.

In the Jacobi method, the old values of v are always used in the right-hand side of Eq. 9.14 until a complete set of new values of v has been computed. Rearranging Eq. 9.10, and letting β mesh aspect ratio = $\Delta x/\Delta y$,

$$v_{i,j}^{k+1} = \frac{1}{2(1+\beta^2)} \left[v_{i+1,j}^{k} + v_{i-1,j}^{k} + \beta^2 v_{i,j-1}^{k} + \beta^2 v_{i,j+1}^{k} - \Delta x^2 f_{i,j} \right] \qquad (9.15)$$

where the superscript, k, refers to the iteration count.

In the Gauss-Seidel method, the most recently available values of v are always used in the right-hand side of Eq. 9.14. That is,

$$v_{i,j}^{k+1} = \frac{1}{2(1+\beta^2)} \left[v_{i+1,j}^{k} + v_{i-1,j}^{k+1} + \beta^2 v_{i,j+1}^{k} + \beta^2 v_{i,j-1}^{k+1} - \Delta x^2 f_{i,j} \right] \qquad (9.16)$$

In the solution of Laplace's equation, the Gauss-Seidel method converges more rapidly than the Jacobi method.

9.5 Successive Overrelation (SOR) Method

Subtracting $v_{i,j}^{k}$ from both sides of Eq. (9.16) and regrouping gives

$$v_{i,j}^{k+1} - v_{i,j}^{k} = \frac{1}{2(1+\beta^2)} \left[v_{i+1,j}^{k} + v_{i-1,j}^{k+1} + \beta^2 v_{i,j+1}^{k} + \beta^2 v_{i,j-1}^{k+1} \right.$$

$$\left. - \Delta x^2 f_{i,j} - 2(1+\beta^2)\, v_{i,j}^{k} \right] \qquad (9.17)$$

Denote the right hand side of Eq. 9.17 by $r_{i,j}$, the residual. Then

$$r_{ij} = v_{i,j}^{k+1} - v_{i,j}^{k}$$

As $v_{i,j}^{k}$ approaches $v_{i,j}^{k+1}$, $r_{i,j}$ approaches zero. Therefore $r_{i,j}$ is a measure of how much the present estimate is in error at (i,j). In the SOR method, the residual is multiplied by a relaxation factor ω. That is,

$$v_{i,j}^{k+1} = v_{i,j}^{k} + \omega r_{i,j} \qquad (9.18)$$

For $\omega=1$, the procedure is identical to the Gauss-Seidel method. However, for a choice of ω in the range of $1<\omega<2$, convergence is more rapid. Depending on the mesh size, the shape of the domain, the type of boundary conditions, an "optimum" value ω_o based on the asymptotic reduction of the most resistant error can be found.

9.6 Alternating Direction Implicit (ADI) Method

By noting that the solution of the elliptic equation may be regarded as the limiting solution (for long times) of the corresponding time-dependent initial value parabolic problem, the solution to $u_t = u_{xx} + u_{yy} - f$ is sought instead. Successive time steps of the solution may be viewed as successive steps of iteration in the elliptic problem. The boundary conditions are identical for both cases. Using the alternating direction implicit method of Peaceman and Rachford, two finite difference equations are obtained.

$$\frac{v_{i,j}^{k+1/2} - v_{i,j}^{k}}{\Delta t/2} = \left[\frac{v_{i+1,j}^{k+1/2} - 2v_{i,j}^{k+1/2} + v_{i-1,j}^{k+1/2}}{\Delta x^2} + \frac{v_{i,j+1}^{k} - 2v_{i,j}^{k} + v_{i,j-1}^{k}}{\Delta y^2} - f_{i,j}\right] \tag{9.19}$$

$$\frac{v_{i,j}^{k+1} - v_{i,j}^{k+1/2}}{\Delta t/2} = \left[\frac{v_{i+1,j}^{k+1/2} - 2v_{i,j}^{k+1/2} + v_{i-1,j}^{k+1/2}}{\Delta x^2} + \frac{v_{i,j+1}^{k+1} - 2v_{i,j}^{k+1} + v_{i,j-1}^{k+1}}{\Delta y^2} - f_{i,j}\right] \tag{9.20}$$

Rearranging, letting the $\Delta x=\Delta y=a$, and the iteration parameter, $\rho = \frac{2a^2}{\Delta t}$,

$$v_{i+1,j}^{k+1/2} - (2+\rho)v_{i,j}^{k+1/2} + v_{i-1,j}^{k+1/2} = -\left[v_{i,j+1}^{k} - (2-\rho)v_{i,j}^{k} + v_{i,j-1}^{k}\right] + a^2 f_{i,j} \tag{9.21}$$

$$v_{i,j+1}^{k} - (2+\rho)v_{i,j}^{k} + v_{i,j-1}^{k} = -\left[v_{i+1,j}^{k+1/2} - (2-\rho)v_{i,j}^{k+1/2} + v_{i-1,j}^{k+1/2}\right] + a^2 f_{i,j} \tag{9.22}$$

Eq. 9.21 and Eq. 9.22 are implicit in x and y, respectively. The first set of linear equations is solved for the intermediate values $v^{k+1/2}$, which are then used in the solution of second set of linear equations. Note that each set of equations involves a tridiagonal coefficient matrix. Just as in the case of the SOR method, an optimum iteration parameter ρ may be determined. The real strength of the ADI method comes in choosing a sequence of iteration parameters, ρ_k, which replaces ρ in Eq. 9.21 and Eq. 9.22. Methods are available for obtaining "good" or "optimum" sequences.

9.7 Upwind Difference Methods for Steady-State Advection-Diffusion Type Equation

Consider a steady-state advection-diffusion type equation in one dimension,

$$w_x \frac{\partial u}{\partial x} - D \frac{\partial^2 u}{\partial x^2} = 0 \tag{9.23}$$

Approximating the derivatives in the above equation by central difference, the finite difference approximation to Eq. 9.23 can be written as,

$$w_x \left(\frac{v_{i+1} - v_{i-1}}{2\Delta x}\right) = D \left(\frac{v_{i+1} - 2v_i + v_{i-1}}{\Delta x^2}\right) = 0 \tag{9.24}$$

The iterative solution of a system of linear equations like Eq. 9.24 will converge only if certain conditions on the coefficients are satisfied. One way of expressing these conditions is that the coefficient matrix must be diagonally dominant. It can be shown that this requires the absolute value of the coefficient of v_i to be at least as large as the sum of the absolute values of all the other coefficients. For those cases where $|w_x|/D \gg 1$, Eq. 9.24 loses diagonal dominance, usually leading to a loss of stability. A method used to overcome this instability is the upwind differencing or donor-cell technique. A one-sided difference is used for the advection term, the direction being "upwind", i.e. forward if $w_x < 0$ and backward if $w_x > 0$. That is,

$$w_x \left(\frac{v_{i+1} - v_i}{\Delta x}\right) - D \left(\frac{v_{i+1} - 2v_i + v_{i-1}}{\Delta x^2}\right) = 0 \qquad \text{if } w_x < 0 \tag{9.25}$$

$$w_x \left(\frac{v_i - v_{i-1}}{\Delta x}\right) - D \left(\frac{v_{i+1} - 2v_i + v_{i-1}}{\Delta x^2}\right) = 0 \quad \text{if } w_x > 0 \qquad (9.26)$$

It can easily be shown that coefficients of Equations 9.25 and 9.26 satisfy the diagonal dominance requirement. Therefore, iterative solutions to these equations are numerically stable. Similar analysis can be extended to multidimensional situations. However, the above procedure possesses only first order accuracy (truncation errors proportional to Δx). Higher order upwind differencing techniques (Roache, 1972, Chang et al. 1974) are available to improve on the accuracy of the finite difference approximations.

9.8 Galerkin Method and Its Modifications

The traditional Galerkin method is a special case of the method of weighted residuals. The method of weighted residuals is an approximate method which seeks a solution to the exact solution in a global sense. This may be contrasted to a Taylor series expansion which seeks an accurate solution in the small region surrounding a single point in the domain.

Consider the following equation:

$$L(u) = 0 \qquad (9.27)$$

where L is a differential operator and Eq. 9.27 may be an ordinary differential equation or partial differential equation of elliptic, hyperbolic or parabolic type. The solution $u=u(\bar{x})$ is sought within some region R and boundary conditions are specified on S, the boundary of R, namely that

$$N(u) = g(\bar{x}) \qquad (9.28)$$

where N is a differential operator of lower order than L.

The first step is to introduce a trial function.

$$v(\bar{x}) = v_o(\bar{x}) + \sum_{j=1}^{n} a_j h_j(\bar{x}) \tag{9.29}$$

It is hoped that v is close to u, the exact solution, in some sense or can be made so if n is large enough. The trial function is chosen to satisfy the boundary conditions exactly. This is often done by making v_o satisfy the boundary conditions exactly, then the analytic function $h_j(\bar{x})$ satisfy homogeneous boundary conditions. Since the approximate solution should be capable of converging to the exact solution as n approaches infinity, it is important that $h_j(\bar{x})$ are linearly independent and chosen from a set of functions which is complete in the domain of interest. The functional form of $h_j(\bar{x})$ may be suggested by the symmetry of the problem, or a boundary condition, or the exact solution of a related problem.

If Eq. 9.29 is substituted into Eq. 9.27, in general Eq. 9.27 is no longer satisfied and a residual r is obtained.

$$L(v) = r(\bar{x}, a_j) \tag{9.30}$$

The size and distribution of r in the domain can be used to assess the accuracy of the solution. For v to be close to the exact solution, the coefficients, a_j, are selected so that the residual is forced to be zero in an average sense,

$$\int_R r(\bar{x}, a_j)\, W_k(\bar{x}) dx = 0, \quad k=1,2,\ldots,n \tag{9.31}$$

where $W_k(\bar{x})$ represents one member of a family of weighting functions. Since there are only n unknown coefficients, a_1, a_2, ..., a_n, there can only be n equations. Since each equation must be independent, so each $W_k(\bar{x})$ must be an independent function. As n, the number of unknown

coefficients in Eq. 9.29, is increased, the approximate solution is expected to approach the exact solution. Or, the residual, r, is expected to decrease as n increases.

There are various ways to choosing the weighting functions leading to (1) the traditional Galerkin method, (2) the least squares method, (3) the method of moments, and (4) the collocation method.

In the traditional Galerkin method,

$$W_k(\bar{x}) = h_k(\bar{x}) \tag{9.32}$$

i.e. the weighting functions are chosen from the same family as the trial functions in Eq. 9.29. Therefore, the set of weighting functions is a linearly independent and complete set in the region R.

In the least squares method,

$$W_k(\bar{x}) = \frac{\partial r}{\partial a_k}(\bar{x}, a_j) \tag{9.33}$$

This is equivalent to replacing Eq. 9.31 with the requirement that $\int_R r^2 \, d\bar{x}$ is a minimum.

In the method of moments,

$$W_k(\bar{x}) = x^k \tag{9.34}$$

In the collocation method,

$$W_k(\bar{x}) = \delta(\bar{x}-\bar{x}_k) \tag{9.35}$$

where δ is the Dirac delta function. This choice of $W_k(\bar{x})$ reduces Eq. 9.31 to forcing $r(\bar{x}=\bar{x}_k) = 0$.

9.9 An Example - Poisson's Equation

Consider the two-dimensional Poisson's equation in a region R with boundary S,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x,y), \qquad (x,y) \text{ in } R \tag{9.36}$$

with the boundary conditions, $u(x,y) = g(x,y)$, (x,y) on S (9.37)

Substituting the trial function, v, into Eq. 9.36, the residual becomes

$$r = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} - f(x,y) \tag{9.38}$$

Imposing the Galerkin condition of Eq. 9.31 with Eq. 9.32,

$$\iint_R r\, h_j \, dx\, dy = \iint_R \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} - f\right) h_j \, dx\, dy = 0 \tag{9.39}$$

Substituting Eq. 9.29 into Eq. 9.39 and rearranging,

$$\sum_i a_i \iint_R \left(\frac{\partial^2 h_i}{\partial x^2} + \frac{\partial^2 h_i}{\partial y^2}\right) h_j \, dx\, dy = \iint_R \left(f - \frac{\partial^2 v_o}{\partial x^2} - \frac{\partial^2 v_o}{\partial y^2}\right) h_j \, dx\, dy \tag{9.40}$$

Eq. 9.40 is of the simple form,

$$Q\,\bar{a} = \bar{b} \tag{9.41}$$

with $$q_{ij} = \iint_R \left(\frac{\partial^2 h_i}{\partial x^2} + \frac{\partial^2 h_i}{\partial y^2}\right) h_j \, dx\, dy$$

and $$b_i = \iint_R \left(f - \frac{\partial^2 v_o}{\partial x^2} - \frac{\partial^2 v_o}{\partial y^2}\right) h_i \, dx\, dy$$

If the matrix Q is nonsingular, the solution is formally given by

$$\bar{a} = Q^{-1}\,\bar{b} \tag{9.42}$$

9.10 Finite Element Method

One difficulty of the direct application of the Galerkin method is the choice of trial functions that satisfy the essential boundary

conditions and also provide an adequate description of the geometry, material and other characteristics of the problem. Another disadvantage is that the matrix Q is dense, that is it has no obvious zero elements and are ill-conditioned for large n, leading to inefficient and inaccurate numerical algorithms. Consequently, the classical Galerkin method is of limited use. With the advent of high-speed digital computers, the idea of using approximating functions localized in a small region was developed, leading to the finite element method.

The first stage of the method is to divide the region of solution into a finite number of small, non-overlapping regions which are called elements. The elements are connected only at a certain number of discrete points on their common boundaries. These points plus a number of specially chosen points inside the elements are called nodes.

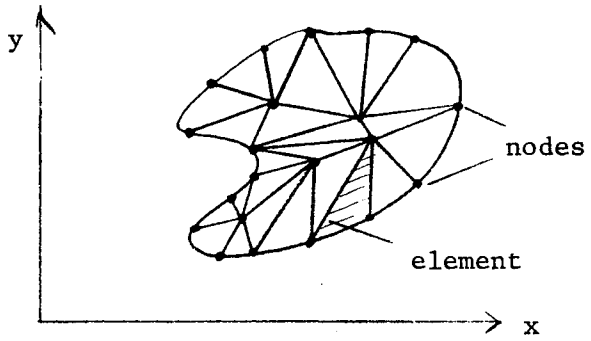

Fig. 9.2 Finite Element Discretization

An approximate solution, defined by,

$$v(\bar{x}) = \sum_{j=1}^{n} N_j(\bar{x}) v_j \qquad (9.43)$$

is introduced. In Eq. 9.43, v_j are the values of v at node j. They replace the unknown coefficients, a_j, in Eq. 9.41, to become the unknowns of the problem. $N_j(\bar{x})$ are referred to as shape functions, with the following property,

$$N_i = 1 \text{ at the } i^{th} \text{ node}$$
$$= 0 \text{ at all other node.} \qquad (9.44)$$

An example of $N_i(\bar{x})$ is shown in Fig. 9.3.

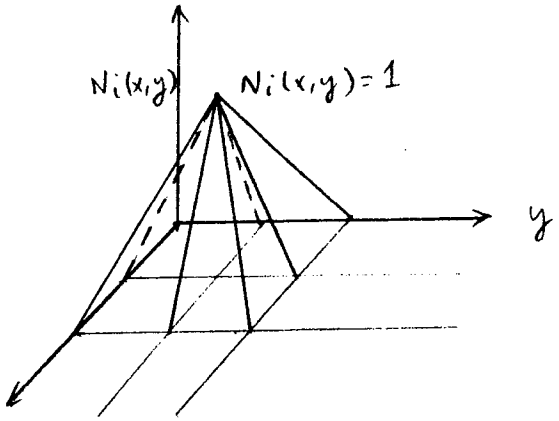

Fig. 9.3 Examples of a Shape Function

Substituting Eq. 9.43 into Eq. 9.31 and Eq. 9.32 and applying boundary conditions, a system of n linear equations with n unknowns is obtained, just as in Eq. 9.41. However, there is one significant difference: because of the localized nature of the shape functions $N_j(\bar{x})$, the only contribution to q_{ij} come from the elements surrounding the i^{th} node. Since the matrix Q is sparse, i.e. there are many zero elements, Eq. 9.41 can be solved economically if the sparse character of Q is taken advantage of.

One significant advantage of the finite element method comes from reducing the integration over the whole domain to the sum of the integrations over individual elements. Using an isoparametric formulation (Zienkiewicz, 1971, Rao, 1982), a regular element can be distorted to an irregular shape to handle arbitrary boundary contours and the corresponding boundary conditions without the need for special procedures.

The convergence of the finite element solution to the exact solution can be brought about in two ways: either the number of nodes per element, i.e. the order of the approximating function, can be increased with the element size fixed or else, by division of the domain into smaller and smaller elements, with the number of nodes per element fixed. In general, there is no fixed rule for determining the optimum element size together with the optimum number of nodes per element. This may have to determined on a case-by-case basis.

If the finite element solution is to converge to the exact solution, the approximating function must satisfy completeness and compatibility conditions for the problem. Let the integrands appearing in the weighted residual Eq. 9.31 contain derivatives up to the m^{th} order. The compatibility condition requires that the shape function and its partial derivatives up to the $(m-1)^{th}$ order must be continuous at element boundaries. The completeness condition requires that the shape function and its partial derivatives up to the m^{th} order must be continuous within each element. Note that it is sometimes possible to reduce the order of the highest derivative appearing in the Eq. 9.31 using integration by parts, or equivalently, using Green's or Stokes' theorems.

9.11 Monte Carlo Method

A Monte Carlo method is any procedure which involves the use of statistical sampling techniques to approximate the solution of a mathematical or physical problem. Monte Carlo methods are not known for all problems nor do specific problems necessarily admit a unique Monte Carlo procedure. There may exist different Monte Carlo methods for a

given problem, not obviously related to one another.

Monte Carlo methods can be used to solve either deterministic or probabilistic problems. The main idea is either to construct a stochastic model which is in agreement with the actual problem analytically, or to simulate the whole problem directly. In both cases, an element of randomness has to be introduced according to well-defined rules. Then a large number of trials or plays is performed, the results are observed, and finally a statistical analysis is undertaken in the usual way. The advantages of the method are that even very difficult problems can often be treated quite easily. The disadvantages are the poor precision and the large number of trials which are necessary.

Monte Carlo methods have been used extensively in various branches of nuclear engineering, e.g. neutron transport, radiation shielding, minimum critical power ratios (Carter and Cashwell, 1975, Thompson and Chen, 1970, Mazumdar 1972, NEDO-10958, 1973). In the present discussion, attention is focused on solving some partial differential equations with Monte Carlo methods. Some familiarity with basic probability concepts is assumed. Thorough treatments may be found in the standard texts, some of which are listed in the references.

9.12 An Example - Laplace's Equation

Consider a particle which is constrained to move on the lattice points with integer coordinates (m,n) in the plane. At each step the particle will move to one of the neighboring lattice points directly above or below or directly to the right or left of the current position. The four possible moves, from (m,n) to (m+1,n), (m-1,n), (m,n+1) or (m,n-1), are each assumed to have probability 1/4. The particle

describes a random path composed of such moves in succession, with the new move randomly determined each time independently of the present position and past history of the particle. Assuming that the particle started at (0,0) there will be defined for each lattice point (m,n) and for each integer k a probability P(m,n,k) that after k steps the particle will be found at (m,n). In order to arrive, after k+1 steps, at (m,n) the particle must have been at one of the four neighbours after the k^{th} step. From each of these positions the probability is 1/4 for the transition of the particle to (m,n). Thus P(m,n,k) satisfies the following linear difference equation

$$P(m,n,k+1) = \frac{1}{4}\,[P(m+1,n,k) + P(m-1,n,k) + P(m,n+1,k) + P(m,n-1,k)] \qquad (9.45)$$

An elementary manipulation transforms Eq. 9.45 to

$$P(m,n,k+1) - P(m,n,k) = \frac{1}{4}\,\{\,[P(m+1,n,k) - 2P(m,n,k) + P(m-1,n,k)] + P(m,n+1,k) - 2P(m,n,k) + P(m,n-1,k)] \qquad (9.46)$$

Observe the similarity of the finite difference equation to the diffusion equation, $P_t = \alpha\,(P_{xx} + P_{yy})$, with first-order forward difference and central differences in x and y with $\Delta x = \Delta y = a$,

$$P(m,n,k+1) - P(m,n,k) = \frac{\alpha\Delta t}{a^2}\,\{\,[P(m+1,n,k) - 2P(m,n,k) + P(m-1,n,k)] + [P(m,n+1,k) - 2P(m,n,k) + P(m,n-1,k)]\,\} \qquad (9.47)$$

which is the same as Eq. 9.47 with $\alpha\Delta t/a^2 = 1/4$.

If instead of starting with a particle at (0,0) for k=0, the process (called a random walk) is started with a probability distribution at (m,n) initially, the function P(m,n,k) may still be interpreted as before and will still satisfy the same difference

equation. The initial distribution of P(m,n,0) correspond to the arbitrary initial function generating a particular solution of Eq. 9.46.

Random behaviour corresponding to the process (random walk) described here may be sampled by establishing an appropriate correspondence between ranges of random numbers and the decisions required at each step. For example, the first draw of a random number may determine the particle's initial point on the lattice, the second may determine the first move, etc. A sequence of such draws will determine a particular path, often referred to as a particle history. A sample of histories of this kind is used to estimate P(m,n,k) for any node (m,n) and for any k to which histories have been carried. The estimate is determined by counting the number of histories for which the corresponding particles are at (m,n) after the k^{th} step and dividing by the sample size.

The statistical process just described is a Monte Carlo process. The determination of random sampling numbers is usually done by generating on the computer a sequence of pseudo-random numbers with a suitable recurrence relation. A relation of the type

$$r_{n+1} = A\, r_n \pmod{m} \qquad (9.48)$$

is often used, where A and m are constants whose optimal choice depends upon the problem and the computer.

Suppose that random walks of the type just described are begun in the interior of a bounded region enclosed by a specific boundary lattice of points (m_i,n_i). For purposes of this discussion, a boundary separates the interior from the exterior of the region by ensuring that any admissible walk, of the type used above, must contain a boundary point on the path between a pair of points, one of which is inside and

the other outside.

The random walks described above will now be modified by terminating any walk upon its first arrival at the boundary. In the language of the physicist, the boundary is an "absorbing boundary" for the particle. It can be proved that the walks eventually terminate in the sense that the probability of remaining forever in the region is zero. Therefore, it is appropriate to attach to any starting point (m,n) a function $P(m_i,n_i,m,n)$ which is the probability that a particle starting at (m,n) terminates its history at boundary point (m_i,n_i). If a function $V(m_i,n_i)$ is initially defined on the boundary, the expected value of U is

$$E(U) = V(m,n) = \sum_i U(m_i,n_i)\, P(m_i,n_i,m,n). \qquad (9.49)$$

In other words, if the value $U(m_i,n_i)$ is attached to all walks terminating at (m_i,n_i), then V(m,n) is the expected terminal value for walks starting at (m,n). Of course, $V(m_i,n_i) = U(m_i,n_i)$. As before V(m,n) satisfies the difference equation

$$V(m,n) = \frac{1}{4}\,[V(m+1,n) + V(m-1,n) + V(m,n+1) + V(m,n-1)] \qquad (9.50)$$

This follows directly from the fact that, of the random walks originating at (m,n), one fourth become new random walks originating at each of the four neighbouring points on the lattice. The analogous differential equation to Eq. 9.50 is Laplace's Equation with Dirichlet boundary conditions specified by U.

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0 \qquad (9.51)$$

This random walk can serve as a basis for the statistical estimation of V(m,n) at a single interior point by starting a number of

particle histories at that point and attaching to each history the value of $U(m_i,n_i)$ assigned to the boundary point (m_i,n_i) where that walk terminates. In this way the method leads to an approximate value to the solution at a single point without carrying out the usual simultaneous solution by direct methods or iteration.

Monte Carlo methods have been employed on a great variety of problems and are especially useful on molecular dynamics, and flow problems. It is not particularly convenient because of the relatively long running times to obtain reasonable answers. However, it is the only feasible method for many complex problems in science and engineering.

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