DISCRETIZATION METHODS FOR PROBLEMS OF MATHEMATICAL PHYSICS

V.I. Agoshkov
Institute of Numerical Mathematics, Russian Academy of Sciences, Moscow, Russia

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Summary

In computational mathematics, the ideas and approaches are aimed at construction and investigation of methods for solving problems of mathematical physics. A feature of these methods is that a problem to be solved is replaced by another one with a finite number of unknown parameters. With a knowledge of these parameters, it is possible to

calculate an approximate solution. Replacing a given problem by a new (but related) one with a finite number of unknowns is called *discretization* and a number of methods may be used for this purpose. Such methods are often called methods for the approximate solution of a given problem.

In this chapter several classes of discretization methods are considered and some theoretical results are presented.

1. Introduction

Often we can solve a problem of mathematical physics only by a numerical method. The construction of algorithms to obtain an *approximate* solution of a problem with specified accuracy is the subject of *computational mathematics.*

Notice that methods of computational mathematics, as a rule, yield approximate results. Another feature of these methods is that calculations can be performed only on a finite number of quantities and a number of obtained results is finite as well. Because of this, a problem to be solved must be reduced to such a form that all results can be obtained in a finite number of arithmetical operations. Replacing a given problem by another (but related) one with a finite number of unknowns is called the discretization of a problem.

Consider some properties which are required of discretization methods (approximate methods of computational mathematics). One of these properties is *consistency* characterizing the accuracy of the approximation of an equation to be solved by a finite system of equations whose solution is assumed to be an approximate solution of an original equation. The study of consistency in discretization methods is closely related to a special field of mathematics called the theory of the approximation of functions which is of great importance in computational mathematics.

Another characteristic of discretization methods is the possibility to find the unknown quantities within prescribed accuracy. Methods satisfying this property are said to be convergent. Let u be an exact solution of a problem. Assume that with the help of some method we obtained a sequence $u_1,\ldots,u_N$ of approximations to u. One of the major problems arising now is to establish the convergence of approximate solutions to the exact one, i.e., whether $u_N \to u$ as $N \to \infty$, and, if this is not always the case, to determine conditions under which the convergence takes place.

Once convergence has been established, we face a more difficult problem concerning the estimation of *the rate of convergence,* i.e., the estimation of how much fast u_N converges to u as $N \to \infty$. For this purpose an estimate of the form $|u - u_N| \le \varepsilon(N)$ called *the error estimate* is often constructed. The rate of convergence is one of the factors that determine computational cost of a method.

One more important property of approximate methods is *numerical stability*. In computation round-off errors may have a dramatic effect on the final results, i.e., the error of approximate solution may increase to a considerable degree. This indicates that a numerical algorithm is unstable. If round-off errors are not accumulated and, hence, have no appreciable effect on results of computations, an algorithm is considered to be stable.

2. Finite Difference Methods

The finite difference methods are among the most popular methods for the numerical solution of various problems of mathematical physics. In these methods, in a domain of a solution a grid is constructed and we look for a solution on this grid. To determine the values of an unknown grid function (i.e., a function defined at nodes of a grid) a system of scalar equations is constructed. A solution of this system is taken to be an approximate solution of a given problem. One way to construct this system of scalar equations is to approximate derivatives, that enter into a differential equation to be solved and into boundary conditions, by difference relations. The name “finite difference methods" arose from this way of discretization.

2.1. The Grid Method

2.1.1. Basic Ideas of the Method

To present basic ideas of the grid method, we begin with its application to a simple linear boundary value problem for an ordinary differential equation.
For $a \le x \le b$ we consider the boundary value problem

$$Au \equiv -u'' + q(x)u = f(x), \quad x \in (a,b), \quad u(a) = u(b) = 0, \tag{1}$$

where $q(x) \ge 0$. Assume that (1) has a unique solution which is continuous on $[a,b]$ and has continuous derivatives up to the fourth order.

The grid method for the problem (1) as well as for many other problems is as follows.

(1) The domain of the differential equation (1) (the segment $[a,b]$) is replaced with some discrete (grid) domain. This means that on $[a,b]$ some points are taken. A set of these points is called *a grid*, although the term normally refers specifically to a domain of dimension more than one.If these points are taken by the rule $x_k = a + kh,\ k = 0,1,\dots,N,\ h = (b-a)/N$ then the grid is said to be uniform. A point x_k is *a node* of the grid.
(2) On the set of nodes of a grid the boundary value problem (1) is replaced by some grid problem. The term grid problem implies some relations between approximate values of a solution of (1) at the nodes. Here, this is a system of linear algebraic equations.
(3) A solution of a grid problem is obtained by using some numerical method; thus approximate values of the solution of the boundary value problem at the nodes of the grid are determined. This is the final objective of the grid method.

We note the following questions being the basic ones in the grid method.

(a) How can we replace the domain of a differential equation (together with the

boundary in the case of a partial differential equation) by some grid domain?
(b) How can we replace a differential equation and boundary conditions by some grid relations?
(c) Will a grid problem be uniquely solvable, stable, and convergent?

We explain the last two terms and give the answers to these questions using the problem (1) as an example.

The construction of a difference scheme. Take a uniform grid

$$x_k = a + kh, \quad k = 0,1,\dots,N, \quad h = (b-a)/N.$$

Consider Eq.(1) at the interior nodes only, i.e., at the points x_k, $k = 1,\dots,N-1$:

$$Au|_{x=x_k} = -u''(x_k) + q(x_k)u(x_k) = f(x_k), \quad k = 1,2,\dots,N-1.$$

Express the derivatives, which enter into the differential equation, in terms of the values $u(x_k)$ at the nodes using the corresponding finite difference relations:

$$u'(x_k) = \frac{u(x_k) - u(x_{k-1})}{h} + r_k^{(1)}(h), \quad r_k^{(1)}(h) = \frac{h}{2}u''(x_k^{(1)}), \quad x_{k-1} < x_k^{(1)} < x_k;$$

$$u'(x_k) = \frac{u(x_{k+1}) - u(x_k)}{h} + r_k^{(2)}(h), \quad r_k^{(2)}(h) = -\frac{h}{2}u''(x_k^{(2)}), \quad x_k < x_k^{(2)} < x_{k+1};$$

$$u'(x_k) = \frac{u(x_{k+1}) - u(x_{k-1})}{2h} + r_k^{(3)}(h), \quad r_k^{(3)}(h) = -\frac{h^2}{6}u'''(x_k^{(3)}),$$

$$x_{k-1} < x_k^{(3)} < x_{k+1};$$

$$u''(x_k) = \frac{u(x_{k+1}) - 2u(x_k) + u(x_{k-1})}{h^2} + r_k^{(4)}(h),$$

$$r_k^{(4)}(h) = -\frac{h^2}{12}u^{IY}(x_k^{(4)}), \quad x_{k-1} < x_k^{(4)} < x_{k+1}.$$

Notice that in the case of more complicated boundary conditions involving $u'(x_0), u'(x_N)$ we can use the following finite difference representations:

$$u'(x_0) = \frac{-u(x_2) + 4u(x_1) - 3u(x_0)}{2h} + O(h^2),$$

$$u'(x_N) = \frac{3u(x_N) - 4u(x_{N-1}) + u(x_{N-2})}{2h} + O(h^2).$$

Taking into account these finite difference relations, for (1) (in this case we use the expression for $u''(x_k)$ only) we obtain

$$Au|_{x=x_k} \equiv A_h u(x_k) - R_k(h) = f(x_k),$$

where

$$A_h u(x_k) = \frac{-u(x_{k-1}) + 2u(x_k) - u(x_{k+1})}{h^2} + q(x_k)u(x_k), \quad R_k(h) = r_k^{(4)}(h).$$

If $R_k(h)$ satisfies the condition $|R_k(h)| \le Mh^2, \quad k = 1,2,\ldots,N-1,$ where $M = \text{const.}$ does not depend on h, then a difference operator A_h is said to be second-order consistent with a differential operator A with respect to h.

Let h be sufficiently small. Then $R_k(h)$ can be neglected to yield

$$A_h u_k = f(x_k), \quad k = 1,2,\ldots,N-1. \tag{2}$$

Under some conditions we can suppose that $u \approx u(x_i),\ i = 0,1,2,\ldots,N$. Generally speaking, we always have $u_i \ne u(x_i)$ and only for $R_k(h) \equiv 0$ it would be expected that $u_i = u(x_i),\ i = 0,1,2,\ldots,N$. The equality (2) is called *a difference scheme* approximating the equation $Au = f(x)$.

Notice that (2) is a system of $N-1$ linear algebraic equations with a triangular matrix. The number of unknowns $u_0, u_1, \ldots, u_N$ is equal to $N+1$.

Taking into consideration the boundary conditions in (1), we get the simplest (in this case) additional equations

$$u_0 = 0, \quad u_N = 0. \tag{3}$$

The formulae (2) and (3) represent a system of $N+1$ linear algebraic equations in unknowns $u_0,\ldots,u_N$. Sometimes (as in the case of the considered problem) some of these unknowns can be determined from the “boundary equations" of the type (3) that results in a problem for $N-1$ unknowns $u_1, u_2, \ldots, u_{N-1}$. In other cases we can express u_0, u_N in terms of $u_1,\ldots,u_{N-1}$ from boundary equations. Substituting these expressions into (3) in place of u_0, u_N, we again arrive at a system of equations in $u_1, u_2, \ldots, u_{N-1}$. It should be noted that in the latter case an operator A_h and right-hand sides in (2) may be modified.

Solving the system (2) and (3) by some algorithm we can expect that $u(x_k) \approx u_k$, $k = 0,1,\ldots,N$.

Solvability of a system of difference equations. In the grid method, an approximate solution of the given problem is calculated as a solution of a system of difference equations.

Let us study solvability of these equations using the system (2) and (3) as an example. Here from the “boundary equations" we have $u_0 = 0, u_N = 0.$ Therefore we consider (2) for $u_1\ldots,u_{N-1}$. If $q(x) \geq q_0 = \text{const} > 0$ then the matrix of (2) has diagonal dominance; for any $\{f(x_k)\}$ the system (2) has a unique solution $\{y_k\}$, moreover,

$$\max_j |y_k| \leq \frac{1}{q_0} \max_k |f(x_k)|.$$

It follows from this inequality that the scheme (2) is *stable* with respect to possible errors in the values $\{f(x_k)\}$.

A solution of (2) can be obtained by well-known *Gauss elimination* which, in the case of a system with a triangular matrix, is also called the *sweep or factorization method*.

Error and convergence estimates for the grid method. We consider these questions for the problem (1). Let $\varepsilon_k = u(x_k) - u_k$, $\varepsilon(h) = \max\limits_{0\leq k\leq N} |\varepsilon_k|$. The grid method is said to be *uniformly convergent*, if $\varepsilon(h) \to 0$ as $h \to 0$. For (1) we have a system of the form

$$A_h \varepsilon_k = R_k(h), \quad k = 1,2,\ldots,N-1, \quad \varepsilon_0 = \varepsilon_N = 0.$$

Assuming that an exact solution of (1) has bounded fourth-order derivatives, we have $|R_k(h)| \leq Mh^2$. Since a matrix of a system for errors $\{\varepsilon_k\}$ has diagonal dominance, we conclude that the estimate

$$\max_k |\varepsilon_k| \leq \frac{1}{q_0} Mh^2 \to 0$$

provides second-order convergence of the grid method in this case.

To study basic problems of the grid method in more complicated cases, various approaches and results developed in the theory of this method (*maximum principle, comparison theorems etc.*) are used.

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Biographical Sketch

Agoshkov Valery Ivanovich is a Doctor of Physical and Mathematical Sciences, professor of Institute of Numerical Mathematics of Russian Academy of Sciences (Moscow). He is the expert in the field of computational and applied mathematics, the theory of boundary problems for the partial differential equations and transport equation, the theory of the conjugate operators and their applications. He is also the author of more than 160 research works, including 9 monographs. His basic research works are devoted to:

- the development of the effective methods of numerical mathematics;
- the theory of Poinkare-Steklov operators and methods of the domain decomposition;
- the development of methods of the optimal control theory and the theory of conjugate equations and their applications in the inverse problems of mathematical physics;
- the development and justification of new iterative algorithms of the inverse problems solution;
- the development of the theory of functional spaces used in the theory of boundary problems for the transport equation;
- the determination of new qualitative properties of the conjugate equations solution.