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COMPACT DIFFERENCE SCHEMES FOR THE DIFFUSION AND SCHRÖDINGER EQUATIONS. APPROXIMATION, STABILITY, CONVERGENCE, EFFECTIVENESS, MONOTONY*

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Abstract

Various compact difference schemes (both old and new, explicit and implicit, one-level and two-level), which approximate the diffusion equation and Schrödinger equation with periodical boundary conditions are constructed by means of the general approach. The results of numerical experiments for various initial data and right hand side are presented. We evaluate the real order of their convergence, as well as their stability, effectiveness, and various kinds of monotony. The optimal Courant number depends on the number of grid knots and on the smoothness of solutions. The competition of various schemes should be organized for the fixed number of arithmetic operations, which are necessary for numerical integration of a given Cauchy problem. This approach to the construction of compact schemes can be developed for numerical solution of various problems of mathematical physics.

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Key words: Compact schemes, Pairs of test functions, Courant number, Two-level scheme, Order of convergence, Effectiveness, Monotony.

1. Introduction

We consider compact difference schemes (or Numerov schemes, high-order compact (HOC) schemes) for the evolution partial differential equations (PDEs):

— the classical diffusion equation:

$$\partial_t u = D\partial_x^2 u + f, \tag{1.1}$$

where $u = u(t, x)$ is the concentration, $f = f(t, x)$ the source term, $D > 0$ the diffusion coefficient, and

— the modified Schrödinger equation

$$\partial_t u = iD\partial_x^2 u + f, \tag{1.2}$$

where $D = \hbar/2m > 0$, $\hbar$ is the Plank constant, m is the mass. We obtain the standard Schrödinger equation from (1.2) if substitute: $f = V(t, x)u$.

We know the Cauchy initial data $u(0, x)$ for the equations, and we want to obtain the solution of the Cauchy problem, i.e., the function $u(t, x)$, $t \in [0, T]$.

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The schemes can be modified for a wide class of PDEs and systems. We consider these two equations as the examples only to avoid sophisticated formulae. We consider various compact approximations of the Cauchy problem for the equations, as well as for the corresponding homogeneous equations, when $f \equiv 0$. We demonstrate the variants of the compact schemes, that much more effective than usual classical schemes. The relevant numerical experiments will be presented below.

2. Test Functions and Compact Schemes

Let us approximate an abstract evolutionary difference equation

$$\partial_t u = Au + f, \tag{2.1}$$

where A is a differential linear operator with respect to spatial variables, by a family of difference relations, that parameterized by the points $\langle t_n,\, x_j\rangle$ of a temporal-spatial difference grid.

The family of the relations ($j = 1, \dots, M,\ n = 0, \dots, N = T/\tau$)

$$\sum_{i\in S(0,u)} \alpha_j^0 u(t_{n+1}, x_{j+i}) + \sum_{i\in S(1,u)} \alpha_j^1 u(t_n, x_{j+i}) = \sum_{i\in S(0,f)} \beta_j^0 f(t_{n+1}, x_{j+i}) + \sum_{i\in S(1,f)} \beta_j^1 f(t_n, x_{j+i}), \tag{2.2}$$

is called one-level scheme. It is called two-level scheme, if the functions $\langle u,\, g\rangle$ in the moment $t = (n+2)\tau$ (where τ is a step with respect to independent variable t) are included into relation (2.2):

$$\sum_{i\in S(0,u)} \alpha_j^0 u(t_{n+2}, x_{j+i}) + \sum_{i\in S(1,u)} \alpha_j^1 u(t_{n+1}, x_{j+i}) + \sum_{i\in S(2,u)} \alpha_j^1 u(t_n, x_{j+i}) = \sum_{i\in S(0,f)} \beta_j^0 f(t_{n+2}, x_{j+i}) + \sum_{i\in S(1,f)} \beta_j^1 f(t_{n+1}, x_{j+i}) + \sum_{i\in S(2,f)} \beta_j^2 f(t_n, x_{j+i}). \tag{2.3}$$

Here $S(m,\, u)$, $S(m,\, f)$ are stencils, α_j^m, β_j^m are coefficients of the scheme. Schemes (2.2) or (2.3) are explicit, if the stencil $S(0,\, u)$ includes the point $x = jh$ only, where h is a spatial step of the scheme. If scheme (2.2) is implicit, we will inverse a matrix Ω_0, which is composed from the coefficients α_j^0 and zeros on every temporal step. The matrix is K-diagonal, where K is equal to the number of the points in the stencil $S(0,\, u)$; $K = 1$ corresponds to the explicit schemes.

The principal question: how should we choice the stencils and the coefficients to obtain a minimal error at the given arithmetic operations number?

Let us consider for every point $(t_n,\, x_j)$ the ideal $\mathbf{I} = \mathbf{I}(G)$ in the ring of the smooth functions of two variables t and x (see, e.g., [1]) which are generated by the functions $u_{k,m}(t,\, x) = (t - t_n)^m (x - x_j)^k$, where $\langle k,\, m\rangle \in G \subset \mathbb{Z}_+ \times \mathbb{Z}_+$. Then the monomials $u_{k,m}$ together with the functions

$$f_{k,m}(t,\, x) = m(t - t_n)^{m-1}(x - x_j)^k - Dk(k-1))(t - t_n)^m (x - x_j)^{k-2},$$

give us the solutions of Eq. (1.1).