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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.

Mathematics subject classification: 65M06.
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 ($j = 1, \dots, M,\ n = 0, \dots, N = T/\tau$)

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

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):

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

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).

If we assume that the pairs $\langle u_{k,m},\ f_{k,\,m}\rangle$ are solutions of (2.2) or (2.3), we obtain the linear homogeneous algebraic equations for the coefficients α_j^m and β_j^m. For instance, we obtain for (2.2) the linear algebraic system

$$\sum_{i\in S(0,u)} \alpha_j^0 u_{k,m}(t_{n+1}, x_{j+i}) + \sum_{i\in S(1,u)} \alpha_j^1 u_{k,m}(t_n, x_{j+i})$$
$$= \sum_{i\in S(0,f)} \beta_j^0 f_{k,m}(t_{n+1}, x_{j+i}) + \sum_{i\in S(1,f)} \beta_j^1 f_{k,m}(t_n, x_{j+i}), \tag{2.4}$$

where $\langle k,\ m\rangle \in G$.

Thus, we use the pairs as test functions for the relevant compact difference scheme construction. The corresponding scheme is parameterized by a pair of the stencils and by a set $G \subset \mathbb{Z}_+ \times \mathbb{Z}_+$. The corresponding examples will be considered below.

Note 2.1. The approach can be developed for the case of the equations with variable coefficients.

Note 2.2. We must check the stability of the obtained scheme in every case. The Fourier transform is useful for the analysis.

Note 2.3. To use implicit difference schemes (CN, CI3, CI3×2 etc) we need to inverse a difference operator at every temporal step. The double-sweep in the one-dimensional case is a most effective. As about implicit compact schemes in a multi-dimensional case, when we need to inverse a block-three diagonal matrix, they are realized by the same tools, that are used for the classic CN scheme: block double-sweep method [4] and iterative approaches (including the multigrid Fedorenko methods and its modifications, see, e.g., [2,3]).

In some special cases (under strong conditions on the computational area, coefficients of the differential equation and boundary conditions) we can use the fast discrete Fourier transform with respect to part of independent variables.

Note 2.4. If we use scheme (2.3), then we need two initial functions, instead of one only for original Eqs. (1.1) or (1.2). We should use the special projection approach for the second initial function construction to conserve the order of approximation with respect to time. See for details [5-7].

Note 2.5. Two-level difference scheme also can be used for approximation of differential Eq. (2.1). The leap-frog scheme $u^{n+1} = 2\tau\,[A_h u^n + f^n] + u^{n-1}$ is, probably, the most famous two-level scheme. To check the stability of a one-level difference scheme with constant coefficients, e.g.,

$$c_1 u_{j-1}^{n+1} + c_2 u_j^{n+1} + c_3 u_{j+1}^{n+1} = c_4 u_{j-1}^n + c_5 u_j^n + c_6 u_{j+1}^n,$$

we apply the Fourier transform to the formula and verify the inequality for the symbol of the scheme:

$$\max_{\xi=1,\ldots,N} |\sigma(\xi)| \le 1 \quad \text{where } \sigma(\xi) = \frac{c_4 \exp(-i\xi h) + c_5 + c_6 \exp(i\xi h)}{c_1 \exp(-i\xi h) + c_2 + c_3 \exp(i\xi h)}; \tag{2.5}$$

sometimes we verify the inequality for all $\xi \in \mathbb{R}$. If $c_1 = c_3$ and $c_4 = c_6$ we can rewrite it:

$$\sigma(\xi) = \frac{2c_4 \cos(\xi h) + c_5}{2c_1 \cos(\xi h) + c_2}.$$

If the coefficients $\{c_j\}_{j=1}^6$ depend on a parameter, e.g., on the Courant number ν, we can obtain from inequality (2.5) a restriction for the parameter.

In the case of a two-level scheme

$$c_1 u_{j-1}^{n+2} + c_2 u_j^{n+2} + c_3 u_{j+1}^{n+2} = c_4 u_{j-1}^{n+1} + c_5 u_j^{n+1} + c_6 u_{j+1}^{n+1} + c_7 u_{j-1}^{n} c_8 u_j^{n} + c_9 u_{j+1}^{n},$$

we consider the eigenvalues $\lambda_{1,2}(\xi)$ of the matrix

$$\begin{pmatrix} \frac{c_4 \exp(-i\xi h)+c_5+c_6\exp(i\xi h)}{c_1 \exp(-i\xi h)+c_2+c_3\exp(i\xi h)} & \frac{c_7 \exp(-i\xi h)+c_8+c_9\exp(i\xi h)}{c_1 \exp(-i\xi h)+c_2+c_3\exp(i\xi h)} \\ 1 & 0 \end{pmatrix}, \tag{2.6}$$

and verify the inequality:

$$\max_{\xi\in\mathbb{R}} |\max \lambda_{1,2}(\xi)| \leq 1, \tag{2.7}$$

or apply the Routh–Hurwitz criterion (after the Joukowsky transform).

The matrix (2.6) has two eigenvectors. One of them describes the diffusion phenomenon, as well as the second eigenvector is an undesirable result of these two layers; see Note 2.4. We should determine additional initial data (two functions instead of one for PDE (2.1)) to minimize the amplitude of the parasitic wave.

Note 2.6. If we solve Eqs (1.1) or (1.2) in a bounded domain, we need a boundary condition. If we use three-point stencil and the Dirichlet boundary condition, we use the boundary conditions together with relations (2.2) or (2.3) for all inner points of the difference grid. If we have some other boundary condition, e.g. the Neumann condition, then we exchange the ideal $\mathbf{I}$ for the boundary points of the grid to obtain high order approximation, i.e. suitable linear algebraic relations on smaller stencils at the points about boundary instead of (2.2) or (2.3). Then we conserve the corresponding order of approximation for the mixed boundary problem.

Note 2.7. If we use a large stencil $S(0, u)$, we must introduce additional boundary conditions with respect to differential mixed problem for (1.1) or (1.2). We should use the special additional numerical boundary conditions to conserve the order of approximation of the scheme with respect to spatial variable.

Note 2.8. If we exchange the basis $\{u_{k,m}\}_{\langle k,m\rangle\in G}$ in the ideal $\mathbf{I}$ on some other one $\{\tilde{u}_q\}_{q\in\tilde{G}}$ and define $\tilde{f}_q = (\partial_t A)\,\tilde{u}_q$, then we obtain another system like (2.3) as well as a compact scheme. However, at $\tau \to 0$, $h \to 0$ the schemes will be equivalent. The choice of the basis may be useful, if the differential operator A with variable coefficients has a singularity at some point x_*. The same problem was solved in [7] by the way, where shallow-water system in spherical coordinate system was approximated by a compact scheme.

Note 2.9. The approach to compact schemes construction with help of test functions sometimes may be exchanged on the Pade approximation approach, see, e.g., [5,6].

3. Numerical Experiments

We verify our schemes on the following solutions at $\in [0, 2\pi]$ with periodical boundary conditions.

3.1. Homogeneous case.

i) $u(0, x) = \cos(x)$, $f \equiv 0$. Then the analytical solution of diffusion Eq. (1.1) is

$$u(t, x) = \exp(-Dt)\cos(x),$$

and of Schrödinger Eq. (1.2) it is

$$u(t,\,x) = \exp(-iDt)\cos(x),$$

i.e., $u = u_* + iu_{**}$; where

$$u_*(t,\,x) = \cos(iDt)\cos(x), \quad u_{**}(t,\,x) = -\sin(iDt)\cos(x).$$

ii) $u_k(0,\,x) = \sin^k(x)\exp(x),\ k = 0,\,\ldots,\,4$ for the diffusion equation and $k = 2,\,3,\,4$ for the Schrödinger equation; $f_k \equiv 0$. The functions $u_0,\ u_1',\ u_2'',\ u_3''',\ u_4^{[iv]}$ are discontinuous at $x = 0 \sim 2\pi$. We do not know the analytical solutions in the cases. Instead of them we use the numerical solutions, which were obtained with a very small step.

3.2. Non-homogeneous case.

The errors of the compact schemes depend on the smoothness of solutions u and right hand sides (forcing) f.

iii) $\tilde{u}(t,\,x) = \cos(x)\sin(t),\ \tilde{f}(t,\,x) = \cos(x)[\cos(t) + D\sin(t)]$ for the diffusion equation and

$$\tilde{u}(t,\,x) = \cos(x)\sin(t), \quad \tilde{f}(t,\,x) = \cos(x)[\cos(t) + iD\sin(t)],$$

for the Schrödinger one.

iv) $u_k^*(t,\,x) = \sin(t)\sin^k(x)\exp(x),\ f_k^*(t,\,x) = \left[\partial_t - D\partial_x^2\right]u_k^*(t,\,x),\ k = 2,\,3,\,4$ for the diffusion equation and $f_k^*(t,\,x) = \left[\partial_t - iD\partial_x^2\right]u_k^*(t,\,x)$ for the Schrödinger one. We do not use the functions at $k = 0,\,1$, because in the cases for all t the right hand sizes $f_k^*(t,\,x)$ are singular at $x = 0$, and the schemes cannot approximate the distributions (generalized functions) on a discrete grid. The jumps amplitude of the second derivative $J = u_2(2\pi) - u_2(0)$ is equal to 1069, and therefore the amplitude of the jump of the forcing f_2 is equal to $1069D$.

Usually a fixed non-dimensional Courant number $\nu = \tau D h^{-2}$ is used for the various difference schemes comparison. However, the optimum is conditional. The optimal Courant number depends not only on the concrete scheme, but on the solution smoothness as well as on the number of knots of the relative temporal-spatial grid; see Sect. 9.

4. Explicit Compact One-Level Scheme and Euler Explicit Scheme

Let us consider the compact explicit scheme which corresponding to Fig. 4.1.

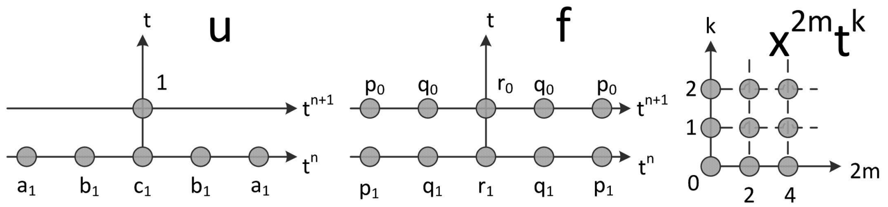

Fig. 4.1. The stencils and the set of the test functions (Newton diagram) for explicit one-level scheme (4.1). The stencil of the classical Euler scheme with operator $A_{h,5}$ for u is the same, and with operator $A_{h,3}$ the stencil is shorter, i.e. $a_1 = 0$.

Then we obtain the following solution of the corresponding algebraic system (2.4):

$$
\begin{aligned}
a_1 &= \frac{\nu(6\nu-1)}{12}, & b_1 &= -\frac{2\nu(3\nu-2)}{3}, \\
c_1 &= 3\nu^2 - 5\nu/2 + 1, & p_0 &= p_1 = \tau\frac{\nu(6\nu-1)}{48}, \\
q_0 &= q_1 = -\tau\frac{\nu(3\nu-2)}{6}, & r_0 &= r_1 = \tau\frac{4-5\nu+6\nu^2}{8},
\end{aligned}
$$

where $\nu = \tau D h^{-2}$ or $\nu = i\tau D h^{-2}$ — the dimensionless Courant parameter (number). If the Courant parameter is fixed, then $\tau = O\left(h^2\right)$ as $h \to 0$. We obtain the compact explicit scheme:

$$
\begin{aligned}
&a_1(u_{-2h,0} + u_{2h,0}) + b_1(u_{-h,0} + u_{h,0}) + c_1 u_{0,0} + u_{0,\tau} \\
=&p_1(f_{-2h,0} + f_{2h,0}) + q_1(f_{-h,0} + f_{h,0}) + r_1 f_{0,0} + p_0(f_{-2h,\tau} + f_{2h,\tau}) + q_0(f_{-h,\tau} + f_{h,\tau}) + r_0 f_{0,\tau}.
\end{aligned} \tag{4.1}
$$

The scheme is stable for diffusion Eq (1.1), if $\nu \leq 2/3$.

The old classic explicit Euler scheme for an arbitrary Eq (2.1) is

$$
u^{n+1} = u^n + \tau\left[A_h u^n + f^n\right], \tag{4.2}
$$

where A_h is a difference approximation of the operator A with respect to the variable x, only. We consider two versions of A_h (with three- and five-points stencils) for comparison with our compact approximation:

$$
\begin{aligned}
A_{h,3}u &= h^{-2}\left[u_{j-1} - 2u_j + u_{j+1}\right], \\
A_{h,5}u &= h^{-2}\left[\frac{-1}{12}u_{j-2} + \frac{4}{3}u_{j-1} - \frac{5}{2}u_j + \frac{4}{3}u_{j+1} - \frac{1}{12}u_{j+2}\right].
\end{aligned}
$$

The Euler scheme E3 (with $A_{h,3}$) is stable, if $\nu \leq 1/2$, and E5 (with $A_{h,5}$), if $\nu \leq 3/8$.

Let us consider the results of computations by the difference schemes for the following data i) (see Sect. 3); $x \in [0, 2\pi]$; periodical boundary conditions; $D = 1,\ T = 10,\ h = h_{eul} = 2\pi/N$.

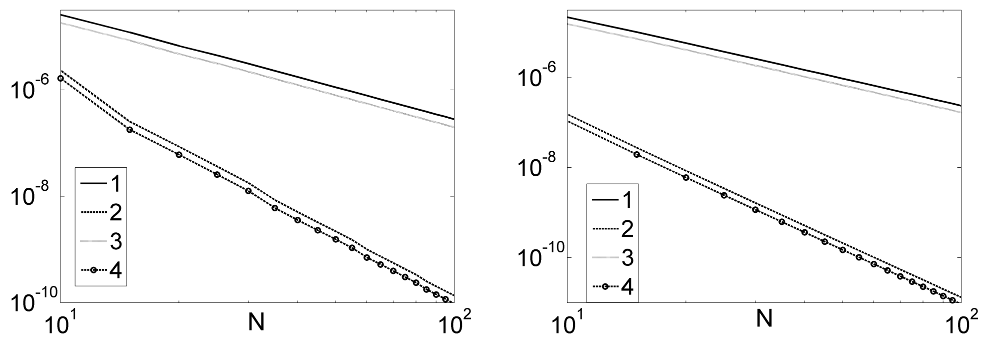

Fig. 4.2. The norms of errors of explicit Euler and compact difference schemes in a bilogarithmic scale. a) 3-point Euler scheme E3 and 5-point explicit compact (C5E) scheme with $h_{comp} = \sqrt[3]{5/3}h_{eul}$; $\nu = 0.48$; b) 5-point Euler scheme E5 and C5E; $\nu = 0.35$ Here the curves: 1 — C-norm error of the corresponding Euler scheme, 2 — C-norm error of the compact scheme, 3 — L^2-norm error of the Euler scheme, 4 — L^2-norm error of the compact scheme.

We compare the compact scheme with 3-point Euler scheme (Fig. 4.2 a) and 5-point one (Fig. 4.2b) for integration of the Cauchy problem for the homogeneous diffusion equation. The 3-point Euler scheme applies 3 multiplications for every knot of the grid against 5 multiplications in the compact scheme. That is why we used in the experiment the compact schemes spatial step $h_{comp} = \sqrt[3]{5/3}h_{eul}$, then the computational time is the same for both schemes. We demonstrate on the Fig. 4.2 the errors evaluation in the norms C and L^2.

The behavior of the errors in C and L^2-norm for various ν is very similar. Also we can see from here that the error of the compact scheme C5E is much less, and it has 4-th approximation order with respect to h against 2-nd order for both Euler schemes E3 and E5.

Note 4.1. The error of approximation of Eq. (2.1) by the formula (4.2) for any spatial approximation A_h (with high order of approximation with respect to x, e.g. 4-th, 6-th, or 8-th) is not better than $\mathbf{O}(\tau)$. If we use a connection between steps $\tau = C_4h^4$, $\tau = C_6h^6$, or $\tau = C_8h^8$, we obtain the high order of approximation. However, such relations lead to very small step τ, and are not effective. If we use the standard relation $\nu = D\tau h^{-2} = \text{const}$, then the total error is estimated as $\mathbf{O}\left(h^2\right)$ as $h \to +0$. Such kind of the schemes comparison with a constant ν is traditional. However, we should find an optimal value ν for every scheme. That is why we firstly fix Q — the number of arithmetic operations (multiplications and divisions only) and minimize the norm of error by the number of steps with respect to space (N) and to time (M). We must take into account that various schemes use the various numbers Q_* of the operations for every knot of a spatial-temporal grid. We obtain here

$$Q = MNQ_*. \tag{4.3}$$

Certainly the numbers Q_* are different for homogeneous and non-homogeneous equations. Below (in Sect.9) we will compare various schemes for the given number Q.

5. Two-Level Explicit Schemes

We can enlarge the stencil of the explicit scheme (4.1) by including an additional temporal level in the scheme stencil, see Fig. 5.1. Then we obtain 6 additional parameters in the compact scheme to improve both order of approximation and stability limit of the scheme.

$$\begin{aligned}
&a_2(u_{-2h,0} + u_{2h,0}) + b_2(u_{-h,0} + u_{h,0}) + c_2u_{0,0} + a_1(u_{-2h,\tau} + u_{2h,\tau})\\
&\quad + b_1(u_{-h,\tau} + u_{h,\tau}) + +c_1u_{0,\tau} + u_{0,2\tau}\\
&= p_2(f_{-2h,0} + f_{2h,0}) + q_2(f_{-h,0} + f_{h,0}) + r_2f_{0,0} + p_1(f_{-2h,\tau} + f_{2h,\tau}) + +q_1(f_{-h,\tau} + f_{h,\tau})\\
&\quad + r_1f_{0,\tau} + p_0(f_{-2h,2\tau} + f_{2h,2\tau}) + q_0(f_{-h,2\tau} + f_{h,2\tau}) + r_0f_{0,2\tau}
\end{aligned} \tag{5.1}$$

We compare solutions, which are obtained by two-level compact schemes 1–4, with the similar solutions of one-level compact scheme (4.1) in series of numerical experiments on the test solutions ii), iv) from Sect. 3, at $\nu_{1,\max} = 2/3$ (the stability limit of one-level explicit scheme (4.1)). In homogeneous case, scheme (4.1) uses $Q_* = 5$ multiplications for every value u_j^{n+1} against $Q_* = 10$ in the two-level schemes 1–4. We obtain $Q_* = 15$ and $Q_* = 25$, correspondingly, for the non-homogeneous equation; see Table 9.1.

The method of gradient descent was used for optimization of free parameters. Also we can choose the number of knots N in relation (4.3) for given numbers Q, Q_*.

The results are not clear yet. These two-level explicit schemes are more effective than one-lever one (4.1). However, the optimal coefficients strongly depend on the available number

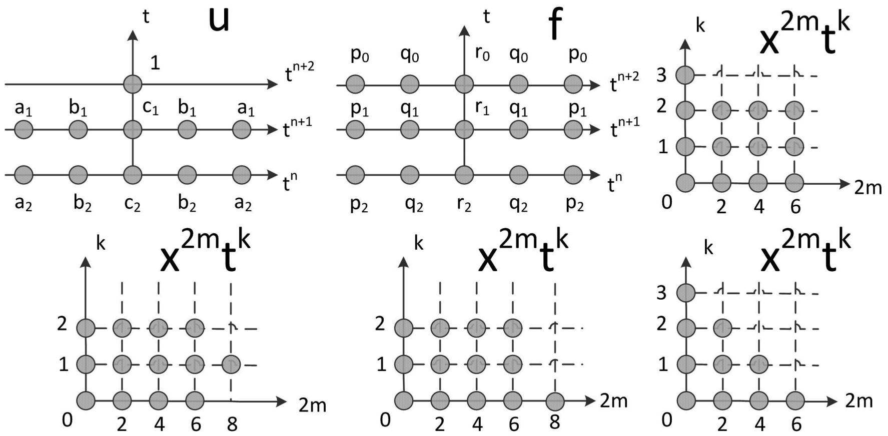

Fig. 5.1. The stencils and the set of the test functions for explicit two-level scheme (5.1). Every Newton diagram generates a compact scheme with free parameters: 2 parameters for the scheme 1, scheme 2, scheme 3 and 5 parameters for scheme 4.

of arithmetic operations, Q, see Table 5.1. The application of such schemes to difference approximations of differential variable coefficients is not clear too.

The coefficients of the scheme (5.1), variant 4 may be optimized in various assumptions and senses with respect to free parameters. We present in the left columns ot Table 5.1 the number of arithmetic operations Q, the minimized norm of the error, and the used test solution. Also we present reaction of the relevant scheme on both test solutions in both norms.

Table 5.1: Q and the minimized norm of the error.

Q	norm	k	err; C; 2	err; L^2; 2	err; C; 4	err; L^2; 4
21000	C	2	**46.62**	32.98	74.05	53.63
21000	L^2	2	25.31	**10.98**	37.17	30.82
21000	C	4	62.07	48.38	**0.52**	0.44
21000	L^2	4	62.34	49.44	0.93	**0.35**
42000	C	2	**21.68**	15.2	35.46	24.88
42000	L^2	2	19.14	**7.02**	31.41	25.27
42000	C	4	46.27	35.85	**0.19**	0.15
42000	L^2	4	43.99	33.9	0.22	**0.12**
84000	C	2	**10.27**	6.38	22.22	20.06
84000	L^2	2	13.66	**4.6**	20.17	17.87
84000	C	4	35.3	27.12	**0.07**	0.05
84000	L^2	4	35.37	27.12	0.08	**0.05**
168000	C	2	**7.57**	4.91	17.24	13.39
168000	L^2	2	12.21	**4.26**	17.81	14.44
168000	C	4	27.72	21.34	**0.03**	0.02
168000	L^2	4	27.93	21.35	0.06	**0.02**

The optimized schemes give us very small integration errors, if we can formulate exactly our goal: an available number of operations, order of smoothness of right hand side and solution, type of norm, where we would like to minimize the error. We use the bold font for the cases.

In other examples the error is larger.

We must mention that the coefficients realize in the space of free parameters $\mathbb{R}^5$ local minima only. In the case of differential equations with variable coefficients this optimization will be very expensive.

6. Implicit Compact One-Level Scheme and Crank–Nicolson Scheme

Let us consider a compact implicit scheme with the stencil like the classical Crank–Nicolson (CN, trapezoidal) scheme, see Fig. 6.1.

We obtain for the compact scheme

$$\begin{aligned} &a_0(u_{-h,\tau}+u_{h,\tau})+b_0u_{0,\tau}+a_1(u_{-h,0}+u_{h,0})+b_1u_{0,0}\\ &=p_0(f_{-h,\tau}+f_{h,\tau})+q_0f_{0,\tau}+p_1(f_{-h,0}+f_{h,0})+q_1f_{0,0}, \end{aligned} \tag{6.1}$$

from the approximation conditions the following coefficients:

$$\begin{aligned} &a_0=2(6\nu-1); \quad a_1=2(6\nu+1); \quad b_0=-4(6\nu+5);\\ &b_1=-4(6\nu-5); \quad p_0=p_1=-\tau; \quad q_0=q_1=-10\tau. \end{aligned}$$

The CN (or trapezoidal) scheme for Eq. (2.1) can be obtained by approximation of differential Eq. (2.1) in the time moment $t=n+1/2$:

$$\frac{u^{n+1}-u^n}{\tau}=\frac{1}{2}\Big(A_h\left(u^{n+1}+u^n\right)+f^{n+1}+f^n\Big).$$

In particular, for differential Eqs. (1.1) and (1.2) CN scheme may be described by the difference equation

$$\frac{u_j^{n+1}-u_j^n}{\tau}=\frac{1}{2}\Big(Dh^{-2}\left[u_{j-1}^{n+1}+u_{j-1}^n-2\left(u_j^{n+1}+u_j^n\right)+u_{j+1}^{n+1}+u_{j+1}^n\right]+f_j^{n+1}+f_j^n\Big), \tag{6.2}$$

and

$$\frac{u_j^{n+1}-u_j^n}{\tau}=\frac{1}{2}\Big(iDh^{-2}\left[u_{j-1}^{n+1}+u_{j-1}^n-2\left(u_j^{n+1}+u_j^n\right)+u_{j+1}^{n+1}+u_{j+1}^n\right]+f_j^{n+1}+f_j^n\Big), \tag{6.3}$$

for standard approximation of the second derivative A_h, correspondingly. However, this operator (not full Eq. (1.1)) may be approximated by the compact scheme $\frac{d^2}{dx^2}\sim\frac{\delta_x^2}{1+\delta_x^2/12}$, (see, e.g., [7,8,11]).

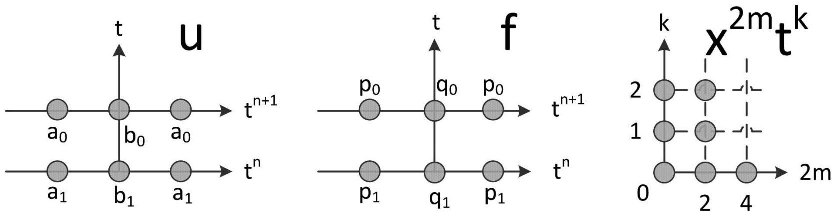

Fig. 6.1. The stencils and the set of the test functions for compact implicit one-level scheme C3I (6.1). The stencil for the Crank–Nicolson scheme for u is the same.

Table 6.1: Errors for CN and the compact sheme C3I.

Scheme	Diffusion equation		Schrödinger equation	
	C	$\mathbf{L}^2$	**C**	$\mathbf{L}^2$
CN	7.69-6	5.44-6	1.10-3	8.09-4
C3I	2.01-8	1.42-8	3.29-6	2.32-6

We search the compact implicit scheme (C3I) for the stencils and the test functions that submitted on Fig. 6.1 in the form

$$\begin{aligned} &a_0(u_{-h,\tau} + u_{h,\tau}) + b_0 u_{0,\tau} + a_1(u_{-h,0} + u_{h,0}) + b_1 u_{0,0} \\ &= p_0(f_{-h,\tau} + f_{h,\tau}) + q_0 f_{0,\tau} + p_1(f_{-h,0} + f_{h,0}) + q_1 f_{0,0}. \end{aligned}$$

We obtain the following coefficients — solution of the system (2.3):

$$\begin{aligned} &a_0 = 2(6\nu - 1); \quad a_1 = 2(6\nu + 1); \quad b_0 = -4(6\nu + 5); \\ &b_1 = -4(6\nu - 5); \quad p_0 = p_1 = -\tau; \quad q_0 = q_1 = -10\tau. \end{aligned}$$

Table 6.1. presents the errors of the classic scheme CN and the compact scheme C3I, when they approximate the diffusion equation and the Schrödinger one. See also Fig. 6.2.

At first we compare the schemes on the smooth test solution i). We can see from the Table 6.1 a significant preference C3I against the classical scheme CN (in 380 times for a) and in 350 times for b)).

Then we consider the Cauchy problem for Eqs. (1.1) and (1.2) with periodic initial function like iii).

Scheme (6.1) is absolutely stable for both Eqs. (1.1), (1.2) and non-dissipative for Eq. (1.2). We can conclude from Fig. 6.3 and Fig. 6.4 that

- 1) the order of approximation for CN scheme is equal to 2, and for the compact scheme it is equal to 4;
- 2) the error of the compact scheme is much smaller for suitable values of the step h.

However, the statement is true for smooth solutions (e.g. for example the solution iv) at $k = 4$) only. We will consider non-smooth tests below.

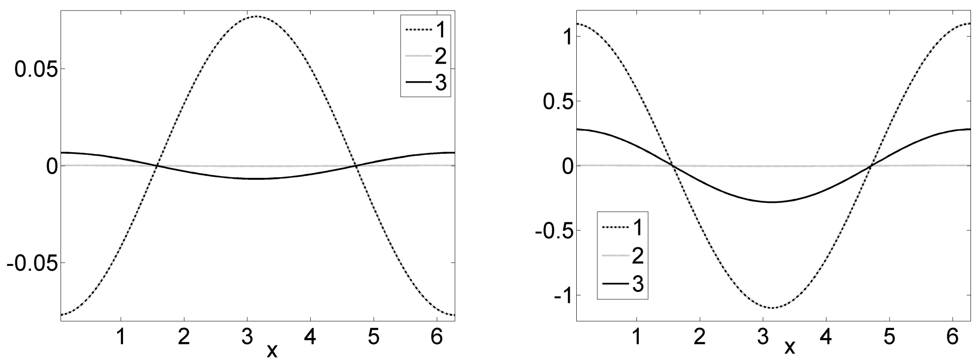

Fig. 6.2. The errors for the homogeneous diffusion equation (a) and for the Schrödinger equation (b) of the schemes CN (curve 1) and C3I (curve 2) multiplied by 10^4 on the a) and by 10^3 on the b). The analytical solution (curve 3) of the Cauchy problem for the test solution i) Sect.3 for a) and real part of the solution for homogeneous Eq. (1.2) for b). Here $N = 120$.

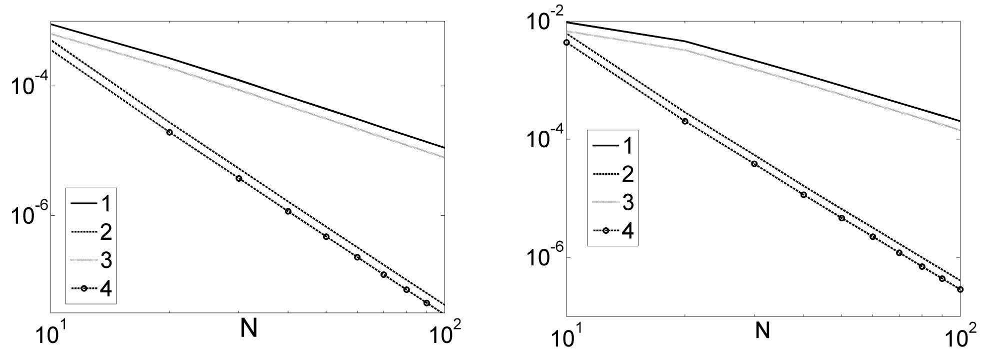

Fig. 6.3. The norms of the errors of the implicit schemes CN and C3I for diffusion Eq. (1.1); $\nu = 1, T = 5$ in the bilogarithmic scale. a) test solution i) in Sect. 3; b) test solution iii) in Sect.3. The curves notations are like Fig. 4.2.

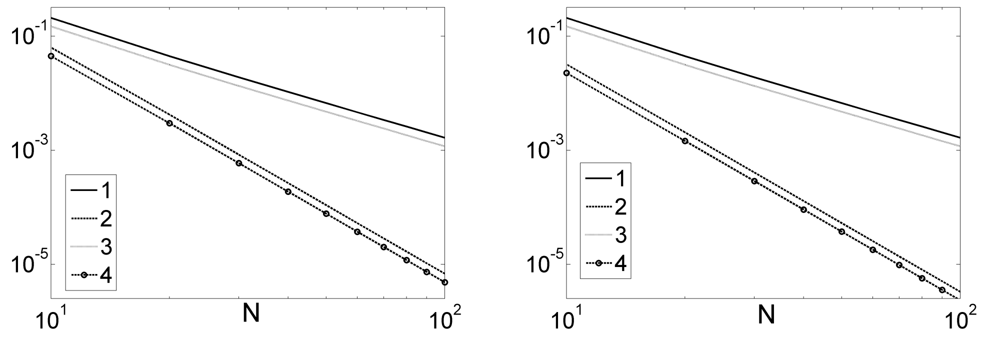

Fig. 6.4. The norms of the errors of implicit CN and compact difference schemes for Schrödinger Eq. (1.2); $\nu = i, : T = 5$ in a bilogarithmic scale. a) test solution i) b) test solution iii). The curves notations are like Fig. 4.2.

7. Implicit Compact Two-Level Scheme

Let us consider the two-level compact scheme with stencils and Newton diagram described on Fig. 7.1. We obtain for the following family of compact schemes

$$\sum_{j=0}^{2} a_j \Big(u(-h, j\tau) + u(h, j\tau) \Big) + b_j u(0, j\tau) = \sum_{j=0}^{2} p_j \Big(f(-h, j\tau) + f(h, j\tau) \Big) + q_j f(0, j\tau). \quad (7.1)$$

Scheme (7.1) is exact for all test functions on Fig. 7.1 at the following coefficients, which depend on two arbitrary real parameters (y, $z \in \mathbb{R}$):

$$a_0 = \frac{1}{10} - \frac{36\nu z}{25\tau}; \quad a_1 = \frac{5y + 10z - 30\nu y + 24\nu z}{25\tau} - \frac{2}{5};$$
$$a_2 = \frac{12\nu}{5} - \frac{10y + 20z + 60\nu y + 216\nu z + 288\nu^2 z}{50\tau} + \frac{3}{10}; \quad b_0 = 1;$$
$$b_1 = \frac{10y + 20z + 12\nu y + 48\nu z}{5\tau} - 4; \quad b_2 = 3 - \frac{-288\nu^2 z - 60y\nu + 50y + 100z}{25\tau} - \frac{24\nu}{5};$$

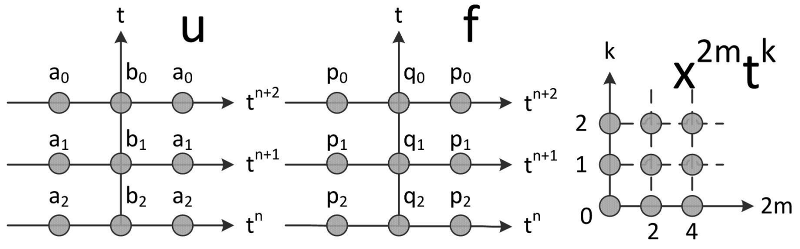

Fig. 7.1. The stencils and the set of the test functions (Newton diagram) for implicit two-level scheme (7.1).

$$
\begin{aligned}
p_0 &= \frac{z}{10}; \quad p_1 = \frac{y}{10}; \quad p_2 = \frac{y}{10} - \frac{\tau}{5} + \frac{3z}{10} + \frac{12\nu z}{25};\\
q_0 &= z; \qquad q_1 = y; \qquad q_2 = y - 2\tau + 3z + \frac{24\nu z}{5}.
\end{aligned} \tag{7.2}
$$

One-level compact scheme (6.1) can be obtained as a particular case of scheme (7.1), (7.2) at $y = z = 5\tau/10 + 12\nu$ or at $y = 0; z = 5\tau/5 + 12\nu$.

However, the stability condition (2.7) for compact schemes (7.1), (7.2) is fulfilled not only for these cases, but for the values $y = 0; z = 5\tau/2(6\nu + 5)$, too. These three compact schemes are absolutely stable both for the diffusion equation and for the Schrödinger equation. They are absolutely stable and non-dissipative for the Schrödinger equation.

Note 7.1. For the last scheme the absolute value of the parasitic eigenvalue is equal to 1 for all wave numbers .

8. Implicit Compact One-Level Scheme with Large Stencils

Let us consider the family of one-level compact schemes with the same stencils and Newton diagram described on Fig. 8.1. We obtain coefficients for the family of compact schemes

$$
\begin{aligned}
&a_0(u_{-2h,0} + u_{2h,0}) + b_0(u_{-h,0} + u_{h,0}) + c_0 u_{0,0} + a_1(u_{-2h,\tau} + u_{2h,\tau}) + b_1(u_{-h,\tau} + u_{h,\tau}) + c_1 u_{0,\tau}\\
&= p_0(f_{-2h,0} + f_{2h,0}) + q_0(f_{-h,0} + f_{h,0}) + r_0 f_{0,0} + p_1(f_{-2h,\tau} + f_{2h,\tau}) + q_1(f_{-h,\tau} + f_{h,\tau}) + r_1 f_{0,\tau},
\end{aligned} \tag{8.1}
$$

but formulae for them are too large to write here.

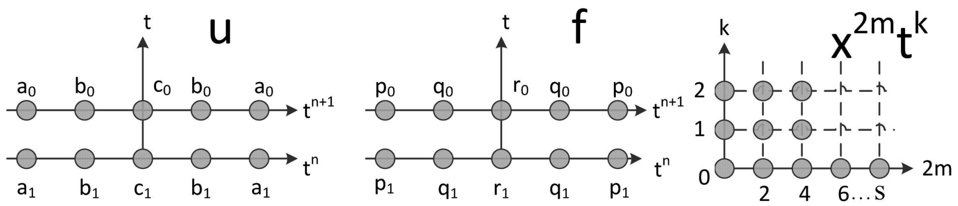

Fig. 8.1. The stencils and the set of the test functions (Newton diagram) for the family of one-level compact schemes (8.1) is a free integer parameter.

Since the coefficients of scheme (8.1) are very close to each other (see Fig. 8.2), let us consider the special case of the family (8.1) only the scheme with stencils and Newton diagram which described on Fig. 8.2.

Table 8.1: Numerical errors on solution ii) ($k = 1$) in Section 3, with $T = 1$ and $\nu = 0.65$ in (1.1).

		Number N				Approximation order			
Scheme	Norm	10	20	40	80	20-10	40-20	80-40	RMS
CI3×2	C	**8.29**	**1.61**	0.33	0.0846	2.37	2.28	1.96	2.21
CI3×2	L^2	**5.26**	0.971	0.205	0.052	2.44	2.24	1.98	2.23
C3I	C	**8.29**	**1.61**	**0.329**	**0.0845**	2.37	2.28	1.96	2.21
C3I	L^2	5.27	0.971	**0.205**	**0.052**	2.44	2.24	1.98	2.23
C5I	C	8.48	1.61	0.33	**0.0845**	2.40	2.28	1.96	2.22
C5I	L^2	5.29	**0.97**	0.206	**0.052**	2.44	2.24	1.98	2.23
C5E	C	16.1	2.29	0.334	0.0847	2.82	2.78	1.98	**2.55**
C5E	L^2	9.22	1.15	**0.205**	0.0521	3.00	2.48	1.98	**2.52**
CN	C	9.10	1.78	0.373	0.0956	2.35	2.26	1.96	2.20
CN	L^2	5.83	1.08	0.223	0.0573	2.42	2.28	1.96	2.23

Table 8.1. presents the results of numerical experiment on solution ii) ($k = 1$) from Sect. 3, with $T = 1$ for various schemes for diffusion Eq. (1.1) with $\nu = 0.65$. Test solution was calculated by scheme (6.1) with 640 knots. The bold font is used here for the best results.

For instance, for the value $s = 4$ we obtain the following coefficients:

$$
\begin{aligned}
&a_0 = -\frac{13402}{477(265\nu+262)} - \frac{31}{318}, && a_1 = \frac{10964}{477(265\nu+262)} - \frac{31}{318},\\
&b_0 = \frac{86768}{477(265\nu+262)} - \frac{64}{159}, && b_1 = \frac{13840}{477(265\nu+262)} - \frac{64}{159},\\
&c_0 = 1,\ c_1 = 1 - \frac{524}{265\nu+262}, && p_0 = p_1 = \frac{23\tau}{18(265\nu+262)},\\
&q_0 = q_1 = \frac{344\tau}{9(265\nu+262)}, && r_0 = r_1 = \frac{131\tau}{265\nu+262}.
\end{aligned} \tag{8.2}
$$

Schemes (8.1) for $s = 4, \dots, 50$ are absolutely stable for Eq. (1.1); they are stable and non-dissipative for Eq. (1.2).

We cannot choose a scheme, which will be unique champion in these tests. The results

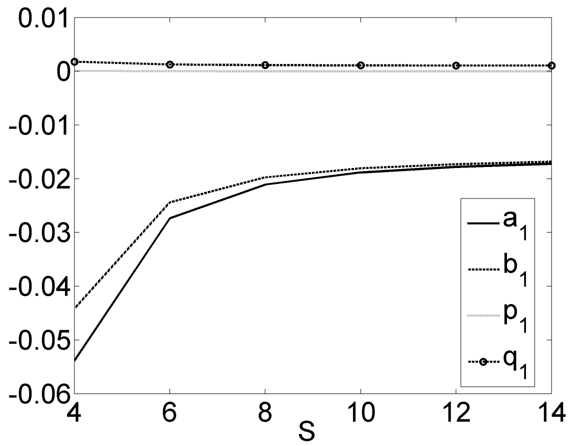

Fig. 8.2. Value of some coefficients of one-level compact scheme (8.1) for $s = 4, \dots, 20$, $\nu = 1$, $\tau = 0.01$.

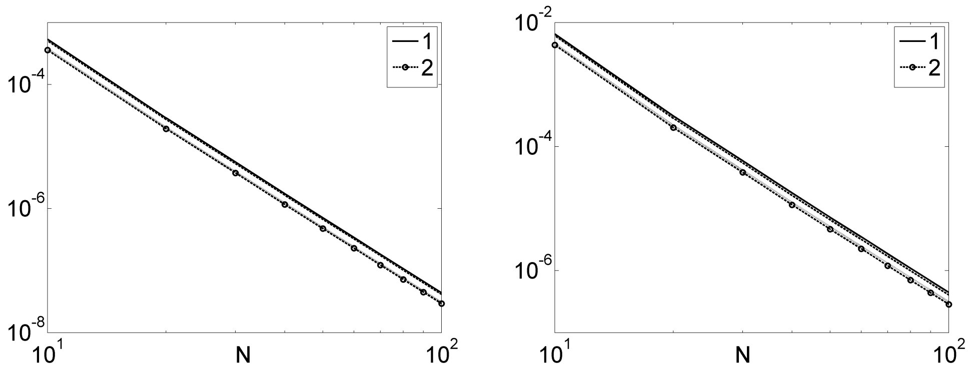

Fig. 8.3. The L^2-norm (curve 1), C-norm (curve 2) of the errors of schemes (8.1)-(8.2) and (6.1) for diffusion Eq. (1.1); $\nu = 1$, $T = 5$, $D = 1$ in a logarithmic scale. a) test solution i); b) test solution iii). The plots of the errors of the schemes (8.1)-(8.2) and (6.1) are equal with a high accuracy.

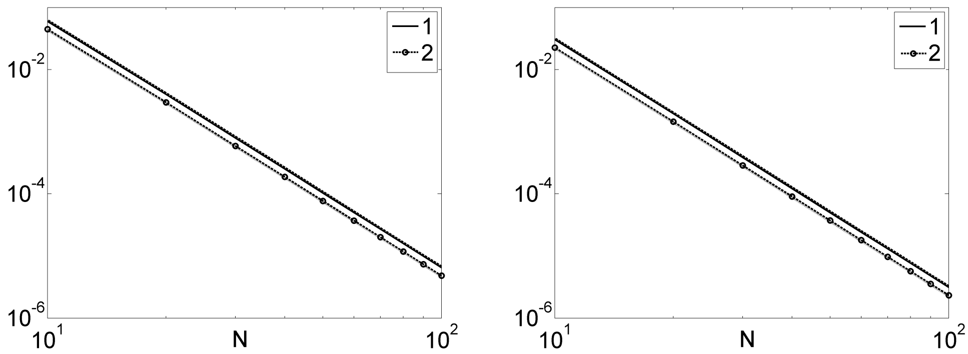

Fig. 8.4. The L^2-norm (curve 1), C-norm (curve 2) of the errors for difference approximations of Schrödinger Eq. 1.2; $\nu = i$, $T = 5$, $D = i$ in a logarithmic scale. Really the errors of scheme (8.1)-(8.2) are equal with a high accuracy to norms of errors of C3I. a) test solution i); b) test solution iii).

depend strongly on the test solutions.

Table 8.2. presents the results of numerical experiment on test solution ii) ($k = 2$) from Sect. 3, with $s = 4, \ldots, 50$ for various schemes for diffusion Eq. (1.1) with $\nu = 0.65$. Test

Table 8.2: Same as Table 8.1, except with $k = 2$.

		Number N				Approximation order			
Scheme	Norm	10	20	40	80	20-10	40-20	80-40	RMS
CI3×2	C	5.65+0	8.45-1	1.25-1	**3.52-2**	2.74	2.76	1.82	2.48
CI3×2	L^2	3.63+0	**5.39-1**	7.88-2	**2.21-2**	2.75	2.77	1.83	2.49
C3I	C	5.65+0	8.46-1	**1.24-1**	**3.52-2**	2.74	2.76	1.82	2.48
C3I	L^2	3.63+0	5.40-1	7.88-2	**2.21-2**	2.75	2.78	1.83	2.49
C5I	C	**5.64+0**	**8.43-1**	**1.24-1**	**3.52-2**	2.74	2.76	1.82	2.48
C5I	L^2	**3.62+0**	**5.39-1**	**7.87-2**	**2.21-2**	2.75	2.77	1.83	2.49
C5E	C	7.34+0	8.75-1	1.27-1	3.53-2	3.07	2.79	1.84	**2.62**
C5E	L^2	4.48+0	5.52-1	7.94-2	2.22-2	3.02	2.80	1.84	**2.60**
CN	C	6.99+0	1.11+0	1.88-1	5.10-2	2.65	2.56	1.88	2.39
CN	L^2	4.16+0	6.65-1	1.10-1	2.99-2	2.65	2.59	1.88	2.40

Table 8.3: Same as Table 8.1, except with $k = 3$.

		Number N				Approximation order			
Scheme	Norm	25	50	100	200	50-25	100-50	20-100	RMS
CI3×2	C	5.15+0	7.82-1	**1.14-1**	**3.22-2**	2.72	2.78	1.83	2.48
CI3×2	L^2	3.33+0	4.95-1	7.24-2	**2.03-2**	2.75	2.77	1.83	2.49
C3I	C	5.15+0	7.82-1	**1.14-1**	**3.22-2**	2.72	2.78	1.82	2.48
C3I	L^2	3.33+0	4.94-1	7.23-2	**2.03-2**	2.75	2.77	1.83	2.49
C5I	C	**4.94+0**	**7.79-1**	**1.14-1**	**3.22-2**	2.66	2.77	1.82	2.46
C5I	L^2	**3.32+0**	**4.94-1**	**7.23-2**	**2.03-2**	2.75	2.77	1.83	2.49
C5E	C	1.03+1	8.56-1	1.16-1	**3.23-2**	3.59	2.88	1.84	**2.86**
C5E	L^2	4.03+0	5.06-1	7.29-2	2.04-2	2.99	2.79	1.84	**2.59**
CN	C	6.50+0	1.02+0	1.71-1	4.64-2	2.67	2.57	1.88	2.40
CN	L^2	3.80+0	6.09-1	1.01-1	2.74-2	2.64	2.59	1.88	2.40

Table 8.4: Numerical errors on solution ii) ($k = 2$) in section 3, with $T = 10$, and $\nu = i$ in (1.2).

		Number N				Approximation order			
Scheme	Norm	25	50	100	200	50-25	100-50	20-100	RMS
CI3×2	C	4.23+1	2.20+1	4.74+0	1.31+0	0.94	2.21	1.85	1.75
CI3×2	L^2	2.92+1	1.09+1	3.04+0	9.67-1	1.41	1.84	1.65	1.66
C3I	C	3.02+1	9.07+0	3.13+0	7.14-1	1.73	1.53	3.12	**1.82**
C3I	L^2	2.23+1	6.67+0	1.76+0	5.27-1	1.74	1.92	1.74	**1.80**
C5I	C	**3.01+1**	**8.96+0**	**2.87+0**	**8.94-1**	1.75	1.64	1.68	1.69
C5I	L^2	**2.17+1**	**6.73+0**	**1.72+0**	**5.15-1**	1.69	1.97	1.74	**1.80**
CN	C	3.90+1	3.21+1	9.42+0	4.84+0	0.28	1.77	0.60	1.17
CN	L^2	2.92+1	1.59+1	6.68+0	2.66+0	0.87	1.25	1.33	1.17

solution is calculated by scheme (6.1) with 640 knots.

Table 8.3. presents the results of numerical experiment on test solution ii) ($k = 3$) from Sect. 3, with $T = 1$ for various schemes for diffusion Eq. (1.1) with $\nu = 0.65$. Test solution is calculated by scheme (6.1) on 640 knots.

Table 8.4. presents the results of numerical experiment on test solution ii) ($k = 2$) from Sect. 3, with $T = 10$ for various schemes for Schrödinger Eq. (1.2) with $\nu = i$. Test solution is calculated by scheme (6.1) on 320 knots.

Table 8.5. presents results of numerical experiment on the test solution ii) ($k = 3$) from Sect. 3, with $T = 10$ for various schemes for Schrödinger Eq. (1.2) with $\nu = i$. Test solution is calculated by scheme (6.1) on 320 knots.

Table 8.5: Same as Table 8.4, with $k = 3$.

		Number N				Approximation order			
Scheme	Norm	25	50	100	200	50-25	100-50	20-100	RMS
CI3×2	C	5.16+1	2.32+1	3.26+0	5.08-1	1.15	2.83	2.68	2.35
CI3×2	L^2	2.92+1	1.20+1	2.13+0	3.66-1	1.28	2.49	2.54	2.18
C3I	C	**3.11+1**	8.97+0	1.73+0	**2.01-1**	1.80	2.37	3.10	**2.48**
C3I	L^2	2.59+1	5.95+0	9.03-1	1.53-1	2.12	2.72	2.56	2.48
C5I	C	3.38+1	**8.73+0**	**1.60+0**	2.26-1	1.95	2.44	2.83	2.44
C5I	L^2	**2.54+1**	**5.86+0**	**8.72-1**	**1.48-1**	2.11	2.75	2.55	**2.49**
CN	C	3.52+1	3.52+1	7.99+0	2.90+0	0	2.13	1.46	1.49
CN	L^2	**2.54+1**	1.78+1	6.22+0	1.88+0	0.51	1.52	1.73	1.36

Table 8.6: Same as Table 8.4, with $k = 4$.

		Number N				Approximation order			
Scheme	Norm	25	50	100	200	50-25	100-50	20-100	RMS
CI3×2	C	4.23+1	2.66+1	3.71+0	3.89-1	0.66	2.84	3.25	2.52
CI3×2	L^2	2.96+1	1.48+1	2.45+0	2.45-1	1.00	2.59	3.32	2.50
C3I	C	3.67+1	**1.16+1**	1.72+0	1.26-1	1.66	2.75	3.77	2.86
C3I	L^2	2.57+1	7.58+0	8.13-1	7.68-2	1.76	3.22	3.40	2.89
C5I	C	**3.38+1**	**1.16+1**	**1.62+0**	**1.13-1**	1.55	2.84	3.84	**2.90**
C5I	L^2	**2.51+1**	**7.40+0**	**7.80-1**	**7.36-2**	1.76	3.25	3.40	**2.90**
CN	C	3.97+1	3.65+1	9.88+0	3.44+0	0.12	1.88	1.52	1.40
CN	L^2	2.75+1	1.94+1	7.60+0	2.10+0	0.50	1.35	1.85	1.36

Table 8.6. presents results of numerical experiment on the test solution ii) ($k = 4$) from Sect. 3, with $T = 10$ for various schemes for Schrödinger Eq. (1.2) with $\nu = i$. Test solution is calculated by scheme (6.1) on 320 knots.

As can be seen from Tables 8.1 – 8.3, schemes CI3×2, C3I, C5I, C5E demonstrate same results on solutions from C^1, C^2, and C^3 of Eq. (1.1), but the order of approximation for C5E is slighty higher.

As for solutions from from C^1, C^2, and C^3 of Eq. (1.2), numerical experiments (see Tables 8.4 – 8.6) shows that the error is less for scheme C5I, althought scheme C3I demonstrates resembling performance.

9. Effectiveness of Difference Schemes

We conclude that the effectiveness of the explicit compact scheme for integration of Cauchy problem for diffusion Eq. (1.1) is much more than the effectiveness of both versions of Euler scheme for the smooth solution as well as the smooth solutions iii) at $k = 4$, see Fig. 9.1. In opposite for solutions with discontinuity at $k = 2$ the Euler 3-point scheme is more effective.

As about Schrödinger Eq. (1.2), the Euler schemes E3 and E5, as well as the compact explicit scheme C5E are absolutely unstable for it.

The implicit schemes are more effective than explicit ones. They are stable for both types of the equations.

Note.9.1. We take into account in the Table 9.1 multiplications and divisions only.

Note.9.2. As about implicit schemes in the Table 9.1, we include the number of operations in the double-sweep method. We do here $6N$ such operations for every temporal step. However, we can do $3N$ operations of the direct sweep one time and then use the coefficients on every temporal step. Thus, we include in the corresponding column 3 operations only for the schemes C3I and CN.

If we will solve the equation with coefficient D, which depending on time t, $D = D(t)$, then we must take into account all $6N$ operations. We assume here, that $D = \text{const}$.

Table 9.1: The number of arithmetic operations Q_* for one knot of a temporal-spatial grid for various explicit and implicit difference schemes.

Scheme	E3	E5	C5E	C5× 2E	C3I	C5I	CN	C3× 2I
Homogeneous	3	5	5	10	6	15	6	12
Non-homogeneous	4	6	15	25	12	21	6	18

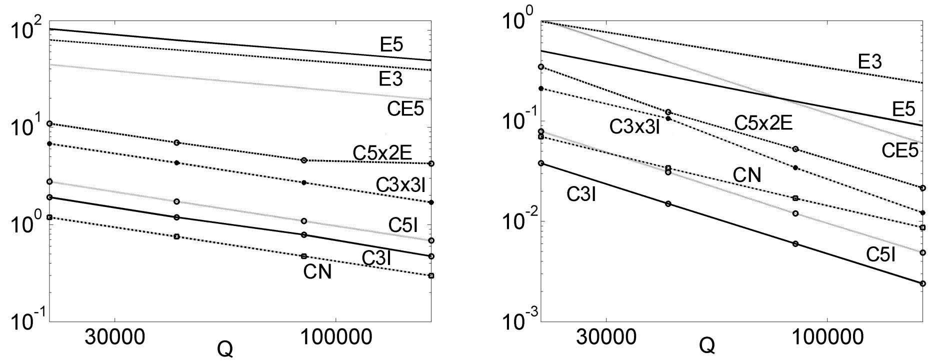

Fig. 9.1. The Cauchy problem integration of the non-homogeneous diffusion equation when the test solution is iv). a) L^2-norm, $k = 2$; b) L^2-norm, $k = 4$. The optimal values of a Courant number ν for various schemes. Bilogarithmic scales.

We twice the numbers for the scheme C5I that uses 5-point double sweep method. Let us consider a difference scheme for Eq. (2.1) and let $\tilde{u}(t)$ be its solution of the Cauchy problem for some given initial data and right hand side. Let us define $E(t) = \|u(t) - \tilde{u}(t)\|$ as a norm of the error. If the estimation

$$E(T) = O\left(S^{-d}\right)$$

as $S \to \infty$ is fulfilled, we define the power d as the order of effectiveness of the scheme.

Certainly, the order depends on the choice of analytical solution $u(t)$ and on the period if integration T. However, it is may be more adequate quantitative characteristic than the orders of approximation and the order of convergence, because the optimal Courant number depends on S. We find the optimal values of all parameters (N and all free parameters of the relative

Table 9.2: The order of effectiveness for various difference schemes, norms and smoothness of test solutions. Approximation of the diffusion equation. The bold font is used here for the best results.

k	2	2	4	4
Norm	C	L^2	C	L^2
E3	0.34	0.35	0.63	0.68
E5	0.36	0.36	0.93	0.82
C5E	0.40	0.40	**1.36**	**1.37**
C5× 2 E	**1.75**	**0.97**	**1.35**	**1.34**
C3I	0.67	0.67	**1.35**	**1.33**
C5I	0.66	0.67	**1.35**	**1.34**
C3× 3 I	0.75	0.67	**1.36**	**1.40**
CN	0.66	0.66	1.01	1.00

Table 9.3: The order of effectiveness for various difference schemes, norms and smoothness of test solutions. Approximation of the Schrödinger equation. The bold font is used here for the best results.

k	2	2	4	4
Norm	C	L^2	C	L^2
C3I	0.59	**0.69**	**1.32**	**1.39**
C5I	**0.68**	**0.67**	**1.35**	**1.39**
C3× 3I	**0.69**	0.65	0.81	0.81
CN	0.57	**0.70**	0.99	0.98

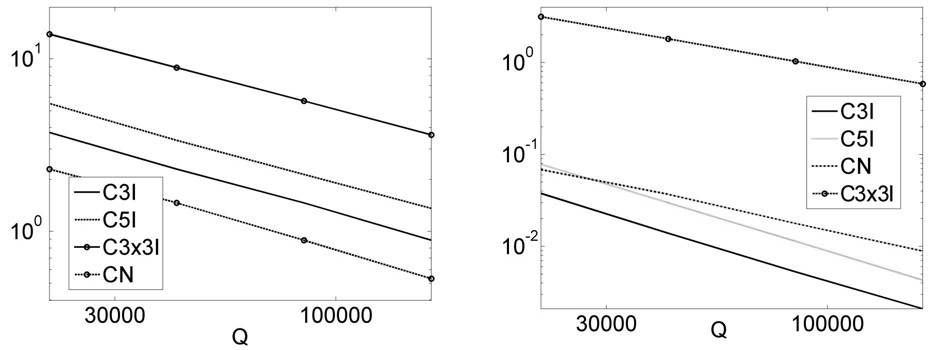

Fig. 9.2. The same results for the Schrödinger equation. Only implicit schemes were considered, because the explicit schemes are unstable.

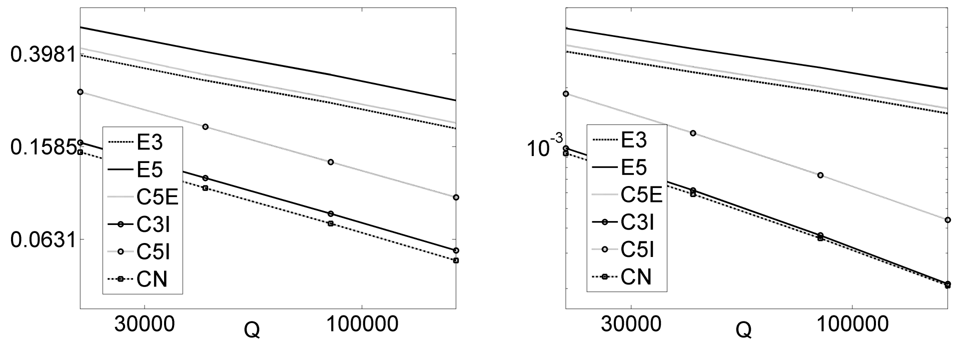

Fig. 9.3. The Cauchy problem integration of the homogeneous diffusion equation when the analytical solution is ii). a) L^2-norm, k=0 b) L^2-norm, $k = 2$. The optimal values of a Courant number ν for various schemes. Bilogarithmic scales.

scheme) for several values Q and then evaluate the order d by least squares method.

Note 9.3. All the schemes are economical according to Samarskii, [10], i.e. the number of arithmetical operations is proportional to the number of knots of the spatial-temporal grid. Also we can estimate the approximation order for these schemes. However, it is not enough for the evaluation of the order of effectiveness, because we optimize the parameters of the scheme

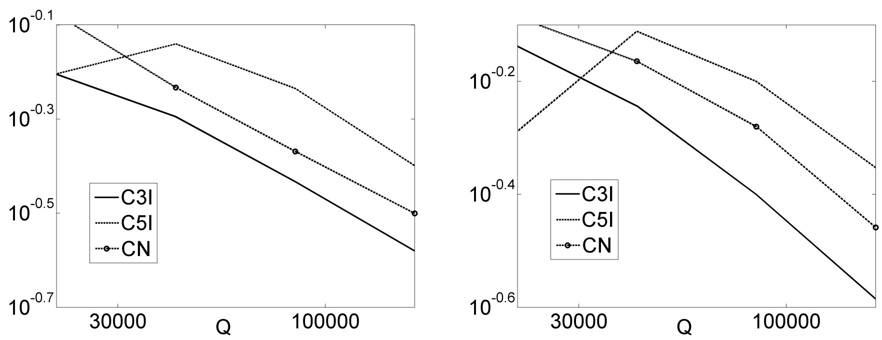

Fig. 9.4. Ibid for the Schrödinger equation. a) L^2-norm, $k = 2$ b) L^2-norm, $k = 4$. Only the implicit schemes described, because the explicit schemes are unstable.

(e.g. its Courant parameter) for any number Q, and the parameters really depend on the value Q. Thus, we evaluate the effectiveness order by numerical experiments.

Thus, the choice of the most effective difference scheme cannot be universal. We obtain from the Tables 8.1–8.6 and 9.2–9.3 that the choice of an optimal scheme from our list should depend on the smoothness of the anticipated solutions. This smoothness can be estimated by the smoothness of the right-hand side of equations (1.1) or (1.2). Probably, the most useful scheme is C3I.

10. Monotony of One-Level Difference Approximations of the Diffusion Equation

The Green function

$$G(t,x,\xi), \quad t>0, \;\; x,\xi \in [0,2\pi],$$

of the periodic mixed boundary problem for homogeneous Eq. (2.1)

$$u\,(0,x) \mapsto u\,(t,x) = \int\limits_0^{2\pi} G(x,\xi,t)u\,(0,\xi)\,d\xi, \quad G(x,\xi,0)=\delta(x-\xi),$$

for homogeneous diffusion Eq. (1.1) at all $t>0$ has the following properties:

i) positiveness: $G(x,\,\xi,\,t)>0$;

ii) symmetry: $G(x,\,\xi,\,t)=G(\xi,\,x,\,t)$;

iii) it has the following unique minimum and maximum:

$$\max_{\xi} G(x,\,\xi,\,t) = G(x,\,x,\,t), \qquad \min_{\xi} G(x,\,\xi,\,t) = G(x,\,x+\pi,\,t);$$

iv) it is strongly decreasing with respect to variable ξ on the segments: $[x,\,x+\pi]\,,[x,\,x-\pi]\,.$

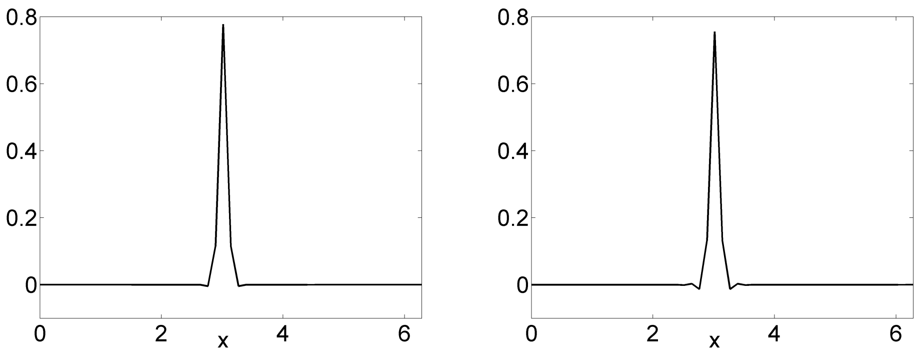

Fig. 10.1. The solution $u(\tau,x)$ of diffusion Eq. (1.1) by the compact schemes a) C3I and b) C5I at $t=\tau$ with $\nu=0.1$ for the Kronecker initial data are not positive. However, negative values are small and they become still smaller for $u(2\tau,x_j)$, $u(3\tau,x_j)$, etc.

In this Sect. we will verify the properties i), iii), iv) for solutions $u(\tau,x_j)$ of the difference schemes with the Kronecker initial data $u(0,x_j)=\delta_0^j$ at $t=\tau$. The property ii) is fulfilled for all considered schemes.

The properties iii) and iv) are fulfilled for the Euler scheme E3 at $\nu \le 1/3$; the property i) at $\nu \le 1/2$. It is equivalent here to the stability condition.

Table 10.1: The limits of various kinds of monotony. The schemes are weakly non-monotonic at $\nu < \nu_1$.

ν	E3	E5	C3I	C5I	CN
ν_1	0	1/6	1/6	0.69	0
ν_2	1/3	17/30	0.53	0.47	0.71
ν_3	1/2	2/3	1.21	1.13	1.49

Table 10.2: The errors (C and L^2norms) of the 3-point implicit schemes for diffusion equation. We use the parameters, which are optimal for effectiveness under the restriction $\nu_1 < \nu < \nu_2$.

Q		21000		42000		84000		168000		336000		772000	
k	Scheme	C	L^2	C	L^2	C	L^2	C	L^2	C	L^2	C	L^2
2	C3I	54.5	42.17	41.95	32.56	31.61	24.46	24.64	19.05	19.30	14.89	14.34	11.05
2	CN	**36.60**	**28.70**	**28.51**	**22.28**	**22.14**	**17.22**	**17.05**	**13.21**	**13.45**	**10.41**	**10.09**	**7.81**
3	C3I	7.71	5.99	4.84	3.77	2.90	2.25	1.84	1.42	1.16	.90	.66	.51
3	CN	**4.61**	**2.98**	**2.89**	**1.87**	**1.81**	**1.16**	**1.10**	**0.71**	**0.7**	**0.45**	**0.40**	**.26**
4	C3I	**0.55**	**0.324**	**0.25**	**0.12**	**0.08**	**0.04**	**0.035**	**0.017**	**0.014**	**0.007**	**0.004**	**0.002**
4	CN	2.12	.86	1.44	0.53	0.90	0.33	0.55	0.20	0.353	0.128	0.202	0.073

The properties i), iii), and iv) are not fulfilled for the Euler scheme E5, since $a_1 = -1/(12h^2) < 0$. The property i) is fulfilled for the compact scheme C5E at $\nu \in [1/6, 2/3]$ only. The inequality

$$u(\tau, x_0) \geq u(\tau, x_0 \pm h)$$

is fulfilled at $\nu \leq 17/30$. Since all the properties i)–iv) are fulfilled on the segment of the Courant number $\nu \in [1/6, 17/30]$ only.

As about one-layer implicit scheme, we can compute numerically for the Kronecker initial data the solution and verify the inequality

$$u(\tau, x_j) \geq 0,$$

for all j. We can use alternatively the discrete Fourier representation for the symbol $\sigma(\xi)$. For instance, we obtain for 3-points stencils:

$$\sigma(\xi) = \frac{b_1 + 2a_1 \cos(\omega)}{b_0 + 2a_0 \cos(\omega)} = \sum_{j=0}^{N-1} \alpha_j \exp(j\omega), \quad \omega = \xi h,$$

since

$$\alpha_j = u(\tau, x_j)$$

at the Kronecker initial data. The coefficients can be calculated by residual theory, too.

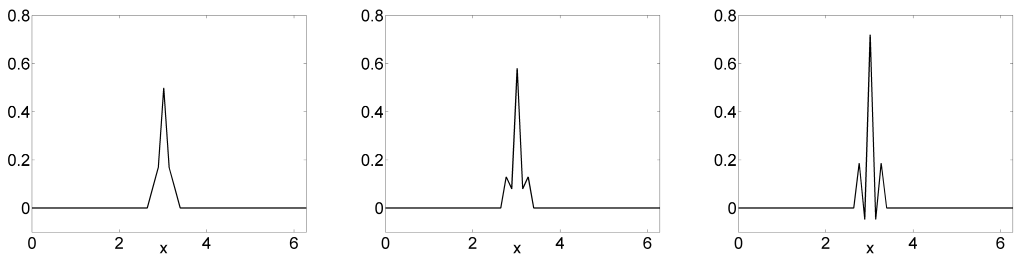

Fig. 10.2. The solution $u(\tau, x_j)$, according to the scheme C5E for the various values of the Courant number: a) $\nu = 0.5$, b) $\nu = 0.6$, c) $\nu = 0.7$.

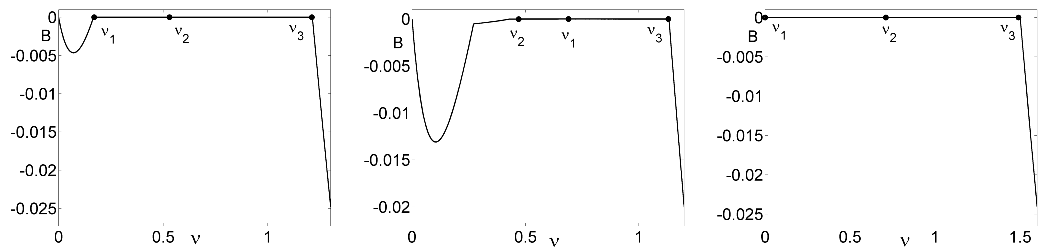

Fig. 10.3. The minimal value of the solution $B(\nu) = \min_j [u(\tau,\, x_j)]$ for implicit schemes for the Kronecker initial data at various values of the Courant number. a) Compact scheme C3I, b) Compact scheme C5I, c) Scheme CN. $N = 50$.

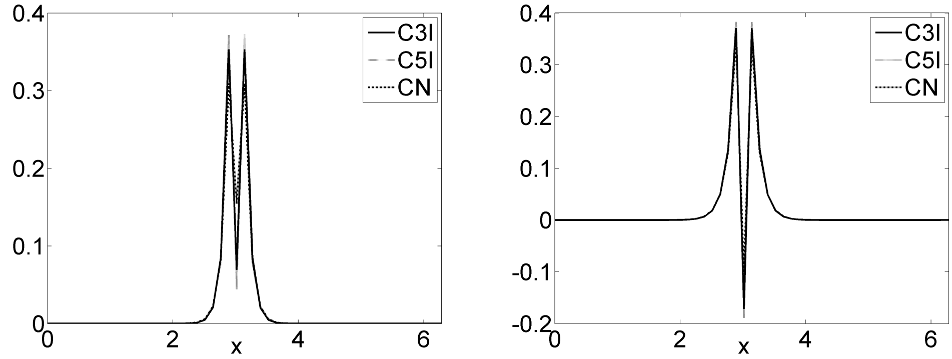

Fig. 10.4. The solutions for implicit schemes at $t = \tau$ are very close a) $\nu = 1$, when $\nu_2 < \nu < \nu_3$; b) $\nu = 2$, when $\nu > \nu_3$. The property $u(\tau,\, x_0) \geq u(\tau,\, x_0 \pm h)$ is not fulfilled. On the right graph the values $u(\tau,\, x_0)$ are negative.

If the Courant number $\nu \ll 1$, then the scheme CN is monotonic unlike the compact schemes C3I and C5I. They have small negative coefficients, see Fig. 10.1 and Table 10.1 at $\nu < \nu_1$. However, the weak effect (weak non-monotony) may be essential for non-smooth solutions only.

The functions $B(\nu) = \min_j [u(\tau,\, x_j)]$ are submitted on the Fig. 10.3. We can see, that the compact schemes are weakly non-monotonic, unlike classical CN scheme. However, the effect is not too essential for practical goals, because the absolute values of the negative coefficients are very small.

The property $u(\tau,\, x_0) \leq u(\tau,\, x_0 \pm h)$ is fulfilled if $\nu \leq \nu_2$. Moreover, at $\nu > \nu_3$ the central value $u(\tau,\, x_0)$ is negative.

The coefficients of the implicit schemes may be estimated. The following asymptotic for

Table 10.3: Same as Table 10.2 except under.

Q		21000		42000		84000		168000		336000		772000	
k	Scheme	C	L^2	C	L^2	C	L^2	C	L^2	C	L^2	C	L^2
2	C3I	38.35	29.72	30.53	23.62	23.36	18.09	18.13	13.98	14.34	11.07	10.71	8.25
2	CN	**27.58**	**21.46**	**21.59**	**16.77**	**17.06**	**13.25**	**13.25**	**10.25**	**10.45**	**8.08**	**7.78**	**6.02**
3	C3I	4.13	3.21	2.73	2.11	1.66	1.29	1.03	.80	.66	.51	.38	.29
3	CN	**2.74**	**1.76**	**1.73**	**1.11**	**1.11**	**0.71**	**0.68**	**0.44**	**0.43**	**0.28**	**0.24**	**0.16**
4	C3I	**0.194**	**0.094**	**0.079**	**0.040**	**0.030**	**0.015**	**0.012**	**0.006**	**0.005**	**0.002**	**0.002**	**0.001**
4	CN	1.36	0.50	0.86	0.32	0.55	0.20	0.34	0.12	0.22	0.08	0.12	0.04

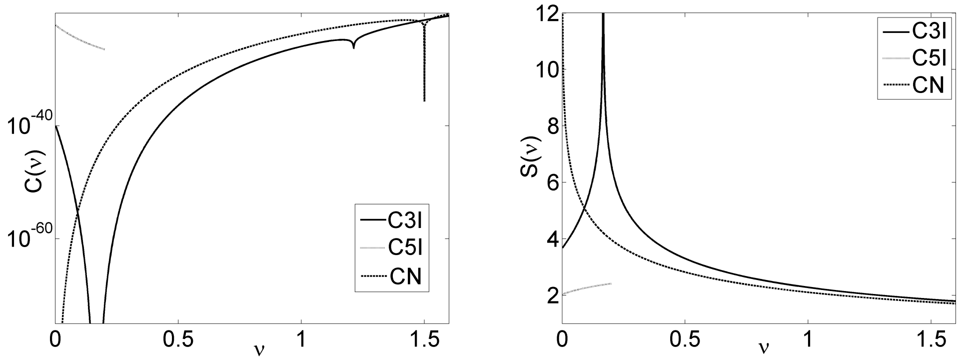

Fig. 10.5. The asymptotics' parameters of the solutions $u(\tau,\, x_j)$ as $j \to \infty$ according to formula (10.1) or (10.2). a) the functions $C(\nu)$; b) the functions $S(\nu)$. The coefficients of C5I satisfy to asymptotic formula (10.1) at small $\nu < 0.2$, only.

$1 \ll j \ll N$:

$$u(\tau,\, x_j) \approx C(\nu)(-1)^{j+1} \exp[S(\nu)|j|] \tag{10.1}$$

is very exact for the scheme C3I at $\nu < \nu_1$ and for the scheme C5I at $\nu < 2$. We call the phenomenon of alternative signs as the weak non-monotony. As about the coefficients of the scheme CN and the scheme C3I at $\nu > \nu_1$, the signs are positive:

$$u(\tau,\, x_j) \approx C(\nu) \exp[S(\nu)|j|]. \tag{10.2}$$

The corresponding functions $C(\nu)$, $S(\nu)$ are represented on the Fig. 10.5.

We evaluated effectiveness of the implicit schemes in the Sect.9. Let us repeat the comparison (on the tests iv)) under the following additional restrictions $\nu_1 < \nu < \nu_2$ or $< \nu < \nu_3$. The results of the experiments see Table 10.2 and 10.3.

11. The Total Probability Conservation for the Homogeneous Schrödinger Equation

The first integral of the homogeneous Schrödinger equation $\int_0^{2\pi} |u(t,\, x)|^2\, dx$ is conserved with time t, if the function $u(t,\, x)$ is a solution of the equation with periodic boundary conditions. All considered explicit schemes are unstable. The implicit schemes C3I, C5I, and CN are stable and non-dissipative: the discrete version of the first integral $\sum\limits_{j=1}^{N} |u(t,\, x_j)|^2$ is conserved with discrete time t with machine precision. We verified it for the test solutions i) and ii) at $k = 2,\, 4$.

12. Summary

We have demonstrated various types of the compact schemes for typical examples of evolutionary linear PDEs (both homogeneous and non-homogeneous): the standard construction algorithm, coefficients, and comparison with the classical difference schemes. A user can choose the suitable compact scheme from the list for his/her concrete computational problem. Usually the relevant compact scheme is preferable. We are going to consider compact schemes for other examples of evolutionary PDE (e.g. equation of rod lateral vibrations) in the next paper.

The classical approach is: two separate algorithms for approximation with respect to time and space. The compact approach is: unite approximation with respect to all variables. We obtain a higher approximation order as the result of compact approach. However, the effectiveness of schemes depends on the assumed test solution smoothness. The approach can be generalized for equations with variable coefficients, for several spatial variables, for systems of equations, and for higher order equations with respect to time.

There are several kinds of monotony restrictions for difference schemes, which approximate the homogeneous diffusion equation. The compact schemes are preferable in comparisons with classic one under such restrictions too.

The implicit compact schemes conserve the discrete analog of the first integral of the homogeneous Schrödinger equation $\int\limits_0^{2\pi} |u(t,\, x)|^2\, dx$ with the computer precision.

Thus, the compact schemes are preferable for a wide class of applied computational problems, and most universal scheme is, perhaps, the implicit scheme C3I.

The important detail is, an accurate approximation of boundary conditions in the mixed problem for a PDE is necessary for the exact approximation of the whole problem.

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