

Solving the Difference Initial-Boundary Value Problems by the Operator Exponential Method

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Received September 19, 2000; Revised February 15, 2001; Accepted March 22, 2001

Abstract

We suggest a modification of the operator exponential method for the numerical solving the difference linear initial boundary value problems. The scheme is based on the representation of the difference operator for given boundary conditions as the perturbation of the same operator for periodic ones. We analyze the error, stability and efficiency of the scheme for a model example of the one-dimensional operator of second difference.

1 Introduction

Numerical solution of the linear difference initial-boundary value problems is an essential part of modelling of the physical processes and phenomena described by the evolutionary differential equations, such as the Schrödinger equation, diffusion equation, Ginzburg–Landau equation and many other.

Along with the classical grid methods [1], an ever increasing use in treatment of such evolutionary problems is currently made of the operator exponential (OE) method [2], which is based on the Lee–Trotter–Kato formula [3] for approximate calculation of the exponential of the sum of noncommuting matrices.

The OE method offers a number of advantages relevant to both explicit and implicit difference schemes. It does not involve iteration procedures and often proves to be absolutely stable. Its applicability is, however, limited by the impossibility to explicitly calculate the exponential of the difference operators expressed in a general form. In fact, effective algorithms of exponential calculation exist only for the difference operators with constant coefficients and periodic boundary conditions on “rectangular” subsets of \mathbb{Z}^n . These algorithms are based on the fast Fourier transform [4] and allow one to calculate the exponential in $O(N \log_2 N)$ operations, where N is the number of points in the domain. For other boundary conditions such algorithms are not available.

In this work a linear difference operator with assigned boundary conditions is considered as perturbation of the same operator with periodic boundary conditions, and the exponential of such an operator is calculated by the Lee–Trotter–Kato formula.

The perturbing operator is essentially an operator in the space of functions on the domain's boundary, so the problem of calculating its exponential is essentially simpler because the number of boundary points is generally much smaller than the total number of points in the domain. This ensures practically the same efficiency of the algorithm proposed as that obtained with the Fourier method for solving the periodic boundary value problems.

Analysis of the error, stability and efficiency of the algorithm proposed is generally quite complicated. So we only present it for a model example of the operator of second difference (one-dimensional difference Laplace operator). This case is probably least "favorable" for the OE method due to availability of effective difference schemes such as the *sweep method* [1]. Nevertheless, the algorithm proposed is competitive with the well-known schemes, in particular, as applied to the Schrödinger equation.

The idea of representing differential operators with various boundary conditions as one another's perturbations was put forward by M G Krein [6] and is being actively used in modern mathematical physics (see, for example, [7]). Applicability of the Krein method to difference operators was considered in [8]. The results of this work were reported at the "Conference on differential equations and applications" (Saransk, Russia, 1994). The summary of this report was published in [5].

2 Description of the method

Let \mathcal{M} be a set of points and $C(\mathcal{M})$ a set of complex-valued functions on \mathcal{M} . Let $\hat{A} : C(\mathcal{M}) \rightarrow C(\mathcal{M})$ be a linear operator of the form

$$(\hat{A}f)(x) = \sum_{y \in \gamma_x} a_x(y)f(y), \quad f \in C(\mathcal{M}), \quad (2.1)$$

where γ_x is a finite subset of \mathcal{M} for each value of x , and $a_x(\cdot)$ is a given function on γ_x .

Let Ω be a subset of \mathcal{M} . We call point $x \in \Omega$ an *inner point* of Ω relative to \hat{A} if $\gamma_x \subseteq \Omega$, and a *boundary point* of Ω relative to \hat{A} if γ_x does not completely lie in Ω . Denote by $\partial_A \Omega$ the set of all boundary points of Ω relative to \hat{A} and let $b_A \Omega = \bigcup_{x \in \partial_A \Omega} \gamma_x \setminus \Omega$.

Note that by definition (2.1), to calculate the values of $\hat{A}f$ at boundary points of Ω , we have to know the values of function f on the set $\Omega \cup b_A \Omega$. A linear operator

$$\hat{L} : C(\Omega) \rightarrow C(\Omega \cup b_A \Omega) \text{ such that } (\hat{L}f)(x) = f(x) \text{ for all } x \in \Omega$$

will be called an *extension operator* for \hat{A} . An operator $\hat{A}_L : C(\Omega) \rightarrow C(\Omega)$ such that $(\hat{A}_L f)(x) = (\hat{A} \hat{L} f)(x)$ for all $x \in \Omega$ will be called an *L-expansion of operator \hat{A}* . The operator \hat{L} plays the same role for difference operators as the boundary conditions play for differential operators.

We now consider a difference initial-boundary value problem for operator \hat{A} :

$$\begin{cases} \frac{\partial f}{\partial t} = \hat{A}_L f, & t \geq 0, \\ f(0, x) = g(x), \end{cases} \quad (2.2)$$

where $f(t, \cdot), g \in C(\Omega)$, \hat{L} is a given extension operator for \hat{A} . The solution of problem (2.2) is of the form:

$$f(t, \cdot) = \exp(t\hat{A}_L)g, \quad (2.3)$$

where operator $\exp(t\hat{A}_L)$ can be defined as a matrix power series since Ω is finite. Given \hat{A} and Ω , the efficiency of computation of $\exp(t\hat{A}_L)$ in (2.3) may largely depend on the extension operator \hat{L} . Let us clarify the above said with a test example.

Let $\mathcal{M} = \mathbb{Z}$, let $\hat{\Delta}$ be the difference Laplacian [1] defined by the relation

$$(\hat{\Delta}f)(x) = f(x-1) - 2f(x) + f(x+1), \quad x \in \mathbb{Z}. \quad (2.4)$$

In this case γ_x in (2.1) is the set $\{x-1, x, x+1\}$,

$$a_x(y) = \begin{cases} 1 & \text{if } y = x-1, \\ -2 & \text{if } y = x, \\ 1 & \text{if } y = x+1. \end{cases}$$

Let $\Omega = \{0, 1, \dots, N-1\}$. Then $\partial_{\Delta}\Omega = \{0, N-1\}$, and $b_{\Delta}\Omega = \{-1, N\}$. Let the extension operator \hat{L} correspond to the periodic boundary conditions for $\hat{\Delta}$:

$$(\hat{L}f)(x) = \begin{cases} f(N-1) & \text{if } x = -1, \\ f(x) & \text{if } x \in \Omega, \\ f(0) & \text{if } x = N. \end{cases} \quad (2.5)$$

The exponential $\exp(t\hat{\Delta}_L)$ in (2.3) can be expressed by the following formula:

$$\exp(t\hat{\Delta}_L) = \hat{F}^{-1} \exp(t\hat{\Lambda})\hat{F}, \quad (2.6)$$

where $\hat{\Lambda}$ is the diagonal operator of the form:

$$(\hat{\Lambda}f)(x) = \nu(x)f(x), \quad \nu(x) = -4 \sin^2 \frac{\pi x}{N}, \quad x \in \Omega,$$

\hat{F} is the operator of the discrete Fourier transform:

$$(\hat{F}f)(x) = \sum_{y \in \Omega} \exp\left(-\frac{i2\pi xy}{N}\right) f(y).$$

Note that computation of the vector $\exp(t\hat{\Delta}_L)f$ via formula (2.6) takes about $N \log_2 N$ operations if we make use of the known Fast Fourier Transform (FFT) algorithm [4].

Let \hat{K} be the extension operator for $\hat{\Delta}$, corresponding to the boundary conditions of the 3rd kind, i.e.,

$$(\hat{K}f)(x) = \begin{cases} \alpha f(0) & \text{if } x = -1, \\ f(x) & \text{if } x \in \Omega, \\ \beta f(N-1) & \text{if } x = N, \end{cases} \quad (2.7)$$

where α and β are, generally, the complex coefficients. (The case $\alpha = \beta = -1$ corresponds to the Dirichlet boundary conditions, and $\alpha = \beta = 1$ to the Neumann boundary conditions.) In this case the known algorithms for exact computation of the vector $\exp(t\hat{\Delta}_K)f$ (for example, using expansion in eigenfunctions of $\hat{\Delta}_K$) involve $\sim N^2$ operations.

Considering the general case again, the question arises: whether the available effective algorithm for the $\exp(t\hat{A}_L)$ computation (\hat{L} is the given extension operator) can be used to approximately evaluate $\exp(t\hat{A}_K)$ for another extension operator \hat{K} ?

Below we describe a version of an OE method which establishes the relation between the exponents of different extensions of a difference operator and thus answer the above question.

Let \hat{K} and \hat{L} be two different extension operators for the operator \hat{A} . We further assume for simplicity that these operators satisfy the following additional condition: the equations $\hat{L}f = \hat{L}g$ and $\hat{K}f = \hat{K}g$ are fulfilled for any $f, g \in C(\Omega)$ such that $f(x) = g(x)$ for $x \in \Omega \setminus \partial_A \Omega$.

Consider operator $\hat{G}_{KL} = \hat{A}_K - \hat{A}_L$. It follows from definition of extension operators, that $(\hat{G}_{KL}f)(x) = 0$ at all inner points $x \in \Omega$, and that $\hat{G}_{KL}f = \hat{G}_{KL}g$ if $f(x) = g(x)$ at the inner points $x \in \Omega$. Therefore, \hat{G}_{KL} is the direct sum of the zero operator in the subspace $C(\Omega \setminus \partial_A \Omega)$ of $C(\Omega)$ and an operator in the subspace $C(\partial_A \Omega)$; we will denote the restriction of \hat{G}_{KL} on $C(\partial_A \Omega)$ by the same character \hat{G}_{KL} .

This suggests that when the number of boundary points of Ω is much smaller than the total number of points in Ω , the problem of computing $\exp(t\hat{G}_{KL})$ becomes much simpler than the initial problem of evaluating $\exp(t\hat{A}_K)$.

Remark. For the extension operators of the general form a small modification of these arguments leads to the same result. In the above example of operator $\hat{\Delta}$ the number of boundary points is equal to two, and the computation reduces to finding the exponential of a 2×2 matrix.

Since $\hat{A}_K = \hat{A}_L + \hat{G}_{KL}$, the following relations hold:

$$\exp(t\hat{A}_K) = \exp(t\hat{A}_L) \exp(t\hat{G}_{KL}) + O(t^2) \equiv \hat{S}_1(t) + O(t^2) \tag{2.8}$$

$$\begin{aligned} \exp(t\hat{A}_K) &= \exp\left(\frac{1}{2}t\hat{G}_{KL}\right) \exp(t\hat{A}_L) \exp\left(\frac{1}{2}t\hat{G}_{KL}\right) + O(t^3) \\ &\equiv \hat{S}_2(t) + O(t^3). \end{aligned} \tag{2.9}$$

They are similar to the conventionally used OE schemes of the 1st and 2nd order approximation [2].

Owing to the above mentioned properties of operator \hat{G}_{KL} , these formulas allow one to roughly calculate the exponential of \hat{A}_K with almost same efficiency as that of $\exp(t\hat{A}_L)$. The natural domain of application of (2.8), (2.9) is the one when \hat{A} is a difference operator with constant coefficients in $C(\mathbb{Z}^s)$, $s \geq 1$ (i.e., the functions $a_x(y)$ in expression (2.1) only depend on the difference $x - y$), and $\Omega = \prod_{j=1}^s \{0, 1, \dots, N_j - 1\}$ is a parallelepiped in \mathbb{Z}^s . In

this case there is a specific extension operator \hat{L} which is defined by the relation $(\hat{L}f)(x) = f(x \bmod N)$, where $(x \bmod N)_j = x_j \bmod N_j$ for $j = 0, 1, \dots, s$, corresponding to the periodic boundary conditions for \hat{A} . The exact value of operator $\exp(t\hat{A}_K)$ is calculated using a multidimensional discrete Fourier transform, the calculation procedure involves about $M \log_2 M$ operations, where $M = N_1 \cdot \dots \cdot N_s$. The number of points of the set $\partial_A \Omega$ can be estimated as

$$|\partial_A \Omega| \leq C(A)M \sum_{j=1}^s \frac{1}{N_j},$$

where the constant $C(A)$ depends on $\#(\text{supp } a(x))$. Hence, if $C(A) \ll \min N_j$, then the size of matrix \hat{G}_{KL} is much smaller than that of \hat{A}_K ; this allows to effectively use formulas (2.8), (2.9). Such a situation occurs in approximations of differential operators with difference ones, and the constant $C(A)$ in this case depends on the order of the operator approximated and, generally, on a method of approximation.

3 Error and stability of the method

Let us now study error and stability of numerical algorithms based on formulas (2.8) and (2.9).

Let $f(t, \cdot) = \exp(t\hat{A}_K)g$ be the exact solution of problem (2.2) with operator \hat{A}_K and $h_j(t, \cdot) = \hat{S}_j(t)g$, $j = 1, 2$, $g \in C(\Omega)$. As an error estimate of one step of the OE algorithms we consider the norms of differences of the functions $f(t, \cdot)$ and $h_j(t, \cdot)$:

$$\varepsilon_j(t, g) = \|f(t, \cdot) - h_j(t, \cdot)\|, \quad j = 1, 2, \quad g \in C(\Omega).$$

By expanding $f - h_j$ in the Taylor series at $t = 0$ we find

$$\varepsilon_1(t, g) = \left\| \left[\hat{A}_K, \hat{G}_{KL} \right] g \right\| \frac{t^2}{2} + O(t^3), \quad (3.1)$$

$$\varepsilon_2(t, g) = \left\| \left(\left[\hat{A}_K, \left[\hat{A}_K, \hat{G}_{KL} \right] \right] - \frac{1}{2} \left[\hat{G}_{KL}, \left[\hat{A}_K, \hat{G}_{KL} \right] \right] \right) g \right\| \frac{t^3}{12} + O(t^4), \quad (3.2)$$

where $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

Thus, the schemes (2.8) and (2.9) have the first and second order of approximation, respectively.

For comparison, consider similar estimates for the classical Euler and Krank-Nickolson (KN) methods [1]. The corresponding approximations are of the form (cf. (2.8) and (2.9))

$$\exp(t\hat{A}_K) = E + t\hat{A}_K + O(t^2) \equiv \hat{S}_e(t) + O(t^2) \quad (3.3)$$

for the Euler scheme and

$$\exp(t\hat{A}_K) = \left(E + \frac{1}{2}t\hat{A}_K \right) \left(E - \frac{1}{2}t\hat{A}_K \right)^{-1} + O(t^3) \equiv \hat{S}_{kn}(t) + O(t^3) \quad (3.4)$$

for the Krank-Nicolson one. It is easy to obtain the estimates for errors of these approximation, namely

$$\delta_1(t, g) = \|\hat{A}_K^2 g\| \frac{t^2}{2} + O(t^3), \quad (3.5)$$

$$\delta_2(t, g) = \|\hat{A}_K^3 g\| \frac{t^3}{12} + O(t^4), \quad (3.6)$$

for Euler and KN schemes, respectively. Clearly, unlike the values δ_j , the estimates ε_j , where $j = 1, 2$, are determined by the norms of commutators of \hat{A}_K with \hat{G}_{KL} , rather than by the powers of \hat{A}_K . This accounts for the differences in the features of the OE algorithms and classical schemes.

Stability analysis of the OE methods (2.8) and (2.9) requires evaluation of the norms of the relevant step operators $\hat{S}_1(t)$ and $\hat{S}_2(t)$. We are going to show that these methods are stable for rather small $t > 0$, if operator \hat{A}_K satisfies the condition

$$\operatorname{Re}(\hat{A}_K g, g) < 0 \quad \text{for any } g \in C(\Omega). \quad (3.7)$$

Indeed, the functions

$$s_j(t, g) = \|\hat{S}_j g\|^2, \quad g \in C(\Omega), \quad \text{for } j = 1, 2$$

are analytic in t in a vicinity of zero, and $s_j(0, g) = \|g\|^2$. Besides,

$$\left. \frac{\partial \hat{S}_j}{\partial t} \right|_{t=0} = 2 \operatorname{Re}(\hat{A}_K g, g) < 0$$

due to the assumption (3.7). Therefore, for a sufficiently small positive values of t the inequality

$$s_j(t, g) = \|g\|^2 + t \left. \frac{\partial \hat{S}_j}{\partial t} \right|_{t=0} + O(t^2) \leq \|g\|^2,$$

is valid, i.e., the schemes (2.8), (2.9) are stable. Note that the condition (3.7) means that the spectrum $\operatorname{spec} \hat{A}_K$ lies in the left half-plane [9]; this guarantees stability of the initial problem (2.2).

There exist two classes of operators \hat{A}_K for which the OE method shows absolute stability.

1. Schemes (2.8), (2.9) are absolutely stable, if \hat{A}_K and \hat{A}_L are Hermitian operators and $\operatorname{spec} \hat{A}_L$ and $\operatorname{spec} \hat{G}_{KL}$ both lie in the left half-plane. This immediately follows from the simplest estimates:

$$\begin{aligned} \|\hat{S}_1(t)\| &\leq \|\exp(t\hat{G}_{KL})\| \|\exp(t\hat{A}_L)\| \leq 1, \\ \|\hat{S}_2(t)\| &\leq \left\| \exp\left(\frac{1}{2}t\hat{G}_{KL}\right) \right\|^2 \|\exp(t\hat{A}_L)\| \leq 1. \end{aligned}$$

This class of operators includes, in particular, the difference Laplace operator with the Dirichlet boundary conditions.

2. The OE method is also absolutely stable, if operators \hat{A}_K and \hat{A}_L are both skew-symmetric, i.e., $\hat{A}_K = -\hat{A}_K^*$ and $\hat{A}_L = -\hat{A}_L^*$. This condition is equivalent to the case when $\operatorname{spec} \hat{A}_K$ and $\operatorname{spec} \hat{A}_L$ both lie on the imaginary axis. Then operators (2.8), (2.9) are unitary (just as the operator $\exp(t\hat{A}_K)$); hence, their norms are equal to 1. An example of such case is the Schrödinger operator.

The OE algorithm may, however, lack absolute stability even when both $\operatorname{spec} \hat{A}_K$ and $\operatorname{spec} \hat{A}_L$ are in the left half-plane. This loss of stability is associated with the positive eigenvalues available for the “boundary” operator \hat{G}_{KL} . The example is a difference Laplacian with the Neumann boundary conditions.

The above estimates can be illustrated by the D -expansion of Laplace operator $\hat{\Delta}_D$ with the extension operator \hat{D} corresponding to the Dirichlet boundary conditions ($\alpha = \beta = -1$ in (2.7)). In this case, as mentioned earlier, schemes (2.8), (2.9) are absolutely stable.

The error estimates for the time step in the OE methods (3.1) and (3.2) depend on the initial vector g . As typical vectors g we consider the eigenfunctions of the operator $\hat{\Delta}_D$:

$$\phi_j(k) = \sqrt{\frac{\sigma_j}{N}} \sin\left(\frac{\pi(j+1)}{N} \left(k + \frac{1}{2}\right)\right), \quad \text{for } j, k = 0, 1, \dots, N-1,$$

where $\sigma_j = 2$, $j = 0, 1, \dots, N-2$; $\sigma_{N-1} = 1$. In this case

$$\varepsilon_1(t, \phi_j) = \begin{cases} 0 & \text{if } j = 1, 3, \dots, N-1, \\ \frac{4t^2}{2\sqrt{N}} \sqrt{-\sigma_j \mu_j (1 + (3 + \mu_j)^2)} + O(t^3) & \text{if } j = 0, 2, \dots, N-2, \end{cases} \quad (3.8)$$

$$\varepsilon_2(t, \phi_j) = \begin{cases} 0 & \text{if } j = 1, 3, \dots, N-1, \\ \frac{t^3}{48\sqrt{N}} \left(-\sigma_j \mu_j (1 + 2(3 + \mu_j)^2) \right. \\ \left. + (\mu_j^2 + 5\mu_j + 7)^2 \right)^{1/2} + O(t^4) & \text{if } j = 0, 2, \dots, N-2, \end{cases} \quad (3.9)$$

where $\mu_j = -4 \sin^2 \frac{\pi(j+1)}{2N}$ for $j = 0, 1, \dots, N-1$, are the eigenvalues of the operator $\hat{\Delta}_D$. The relevant estimates for the Euler (3.3) and KN (3.4) methods are of the form

$$\delta_1(t, g) = \mu_j^2 \frac{t^2}{2} + O(t^3), \quad (3.10)$$

$$\delta_2(t, g) = \mu_j^3 \frac{t^3}{12} + O(t^4). \quad (3.11)$$

Comparing the above estimates we see that, given the same order of approximation, the error of the OE method is much greater for eigenfunctions with small numbers and much smaller for higher harmonics.

Observe that the error in the classical schemes comes from the difference between the eigenvalues of the step operator and $\exp(t\hat{A}_K)$, while their eigenfunctions coincide. The step operators of OE algorithm have error in both the eigenvalues and the eigenfunctions¹. However, as shown numerically, the eigenvalues of the operators $\hat{S}_1(t)$ and $\hat{S}_2(t)$ approximate the spectrum of $\exp(t\hat{A}_K)$ better than the eigenvalues of the classical schemes.

To make sure the above is true, let us find spectrum $\lambda_j(t)$, $j = 0, 1, \dots, N-1$, of the step operator $\hat{S}_2(t)$ for Laplacian $\hat{\Delta}_D$. We show in Appendix that for j odd the eigenvalues and eigenfunctions of operators $\hat{S}_2(t)$ and $\exp(t\hat{\Delta}_D)$ coincide. This is exactly why for these harmonics the errors of the OE methods (3.8) and (3.9) vanish. The remaining $\frac{N}{2}$ eigenvalues are $\lambda_{2j}(t) = \exp(t\xi_j(t))$, $j = 0, 1, \dots, \frac{N}{2}-1$, where $\xi_j(t)$ fulfills the ‘‘dispersion’’ equation (A.9).

The results of numerical solution of this equation are shown in Fig. 1 which provides the values of $|\xi_j - \mu_{2j}|$ as function of j (curve 1).

Clearly, for the majority of harmonics the eigenvalue error of the OE method is much smaller than the error of the KN scheme (curve 2). Besides, one should note the ‘‘uniformity’’ of the spectrum estimate of scheme (2.9): the error weakly depends on the number of the eigenvalues. A similar situation holds also for the operator $i\hat{\Delta}_D$.

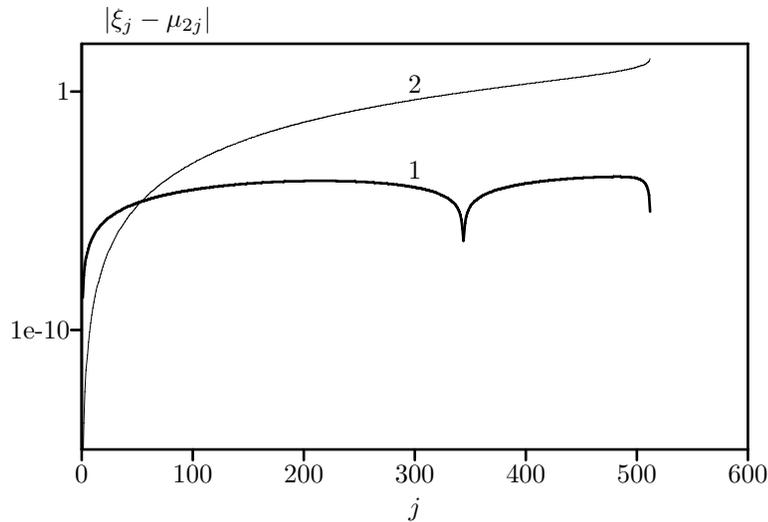


Figure 1. Error in even eigenvalues of step operator for the OE method (1) and the Krank–Nickolson method (2) for one-dimensional Laplace operator with Dirichlet boundary conditions $t = \frac{1}{2}$, $N = 1024$.

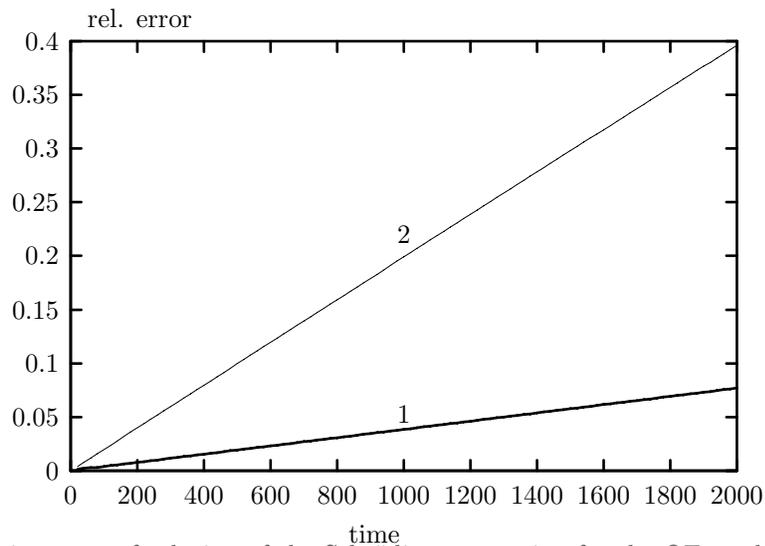


Figure 2. Relative error of solution of the Schrödinger equation for the OE method (1) and the Krank–Nickolson method (2) with random initial vector, $t = \frac{1}{2}$, $N = 128$.

This property of the step operator in the numerical scheme is important when solution of the input evolution problem includes contributions from all eigenfunctions of operator \hat{A}_K . This is the case, for example, in solving problem (2.4) with skew-Hermitian operator \hat{A}_K (Schrödinger equation).

¹It is interesting to observe that the spectra of $\hat{S}_1(t)$ and $\hat{S}_2(t)$ coincide and their eigenfunctions differ only at boundary points.

Fig. 2 shows relative errors of the numerical solution of the problem

$$\frac{\partial f}{\partial t} = i\hat{\Delta}_D f, \quad f(0) = g$$

as a function of time for the OE scheme (2.9) (curve 1) and the Krank–Nickolson one (curve 2). The initial vector g is chosen as a random one; it is uniformly distributed on the unit sphere in \mathbb{C}^N .

4 Conclusion

Splitting methods, including the operator exponential one, are widely used for solving difference linear and quasilinear initial-boundary value problems [2, 4]. The proposed modification of the OE method can be applied when the evolution operator is represented as a sum of a difference operator with constant coefficients on a rectangular domain in \mathbb{Z}^s (the main part) and some, perhaps nonlinear, operator (perturbation). If the boundary conditions for the main part do not allow explicit computation of the input operator exponential, the problem can be approached by a splitting method in two stages: first we split off the perturbation, and then calculate an approximate exponential of the main part using the method proposed in this work.

Consider a rectangular domain in \mathbb{Z}^2 for the Laplacian with boundary conditions of the 3rd kind. Even in this case application of methods like the implicit Euler or Krank–Nickolson schemes requires iteration procedures to obtain the resolvent. The method we propose is explicit and, as follows from the one-dimensional examples provided in the work, competitive with conventional methods.

One of important features of our method is a “uniform” property of the spectral estimate of the initial problem. We have succeeded in applying the scheme described to solve one- and two-dimensional Ginzburg–Landau equation [10], four-order diffusion equation [11] and some other problems.

Appendix

In what follows we derive the equation for the eigenvalues of operator $\hat{S}_2(t)$ defined by relation (2.9) for one-dimensional difference Laplace operator $\hat{\Delta}_D$ with the Dirichlet boundary conditions. To simplify the calculations, we assume that N is even: $N = 2M$.

In this case the “boundary” operator \hat{G}_{KL} is of the form: $\hat{G}_{KL} = -2\hat{Q}_0$, where \hat{Q}_0 is the orthogonal projection on vector $x_0 = \frac{e_1 + e_{N-1}}{\sqrt{2}}$, where $\{e_j\}_{j=0}^{N-1}$ is a standard basis in \mathbb{C}^N . It is easy to calculate the exponential of such an operator:

$$\exp\left(\frac{1}{2}t\hat{G}_{KL}\right) = \hat{E} + (e^{-t} - 1)\hat{Q}_0. \quad (\text{A.1})$$

Let λ be an eigenvalue of $\hat{S}_2(t)$ and Φ_λ the corresponding eigenfunction. Then

$$\hat{S}_2(t)\Phi_\lambda \equiv \exp\left(\frac{1}{2}t\hat{G}_{KL}\right) \exp\left(t\hat{\Delta}_D\right) \exp\left(\frac{1}{2}t\hat{G}_{KL}\right) \Phi_\lambda = \lambda\Phi_\lambda. \quad (\text{A.2})$$

Using expression (A.1) and notation $\Psi_\lambda = \exp\left(\frac{1}{2}t\hat{G}_{KL}\right)\Phi_\lambda$, we express the relation in the form:

$$\left(\lambda\hat{E} - \exp(t\hat{\Delta}_D)\right)\Psi_\lambda = \lambda(1 - e^{2t})\hat{Q}_0\Psi_\lambda. \tag{A.3}$$

Let $\{f_j\}_{j=0}^{N-1}$ be the eigenbasis of operator $\hat{\Delta}_L$ (Laplacian with periodic boundary conditions):

$$(f_j)(k) = \frac{1}{\sqrt{N}} \exp\left(i\frac{2\pi jk}{N}\right), \quad j, k = 0, 1, \dots, N - 1, \tag{A.4}$$

the corresponding eigenvalues ν_j being

$$\nu_j = -4 \sin^2 \frac{\pi j}{N}, \quad j = 0, 1, \dots, N - 1. \tag{A.5}$$

Note that $\nu_j = \nu_{N-j}$ and $\nu_j = \nu_{2j+1}$ for $j = 1, 2, \dots, M$, where μ_k are the eigenvalues of $\hat{\Delta}_D$. Note also that the right hand side of (A.3) for any value of Ψ_λ is proportional to vector x_0 whose expansion with respect to basis (A.4) is:

$$x_0 = \sum_{j=0}^{N-1} (x_0, f_j) f_j = \frac{1}{\sqrt{2N}} \sum_{j=0}^{N-1} \left(1 + \exp\left(-i\frac{2\pi j}{N}\right)\right) f_j. \tag{A.6}$$

If c_j , where $j = 0, 1, \dots, N - 1$, are the expansion coefficients of function Ψ_λ with respect to basis (A.4), then relation (A.3) can be expressed in the form:

$$(\lambda - \exp(t\nu_j))c_j = a_\lambda \lambda (1 - e^{2t})(x_0, f_j), \quad j = 0, 1, \dots, N - 1, \tag{A.7}$$

where $a_\lambda = (\Psi_\lambda, x_0)$.

In order to find all solution of equation (A.6) we consider two cases:

1) $a_\lambda = 0$. In this case $c_j = 0$ or $\lambda = \exp(t\nu_j)$ for each $j = 0, 1, \dots, N - 1$. Since $\Psi_\lambda \neq 0$, there exists index l such that $c_l \neq 0$. In this case $\lambda = \exp(t\nu_l) = \exp(t\nu_{N-l})$ for $l = 1, 2, \dots, M$ and $c_j = 0$ for $j \neq l, N - l$. The corresponding eigenfunctions are found from the condition $a_\lambda = 0$:

$$\Psi_l(k) \sim \sin \frac{2\pi l}{N} \left(k + \frac{1}{2}\right), \quad k = 0, 1, \dots, N - 1, \quad l = 1, 2, \dots, M. \tag{A.8}$$

Note that these functions are the eigenfunctions of operator $\hat{\Delta}_D$ corresponding to the eigenvalues μ_{2l-1} , where $l = 1, 2, \dots, M$.

2) $a_\lambda \neq 0$. In this case $\lambda \neq \exp(t\nu_j)$ for each $j = 0, 1, \dots, N - 1$ as follows from (A.7). Multiplying both sides of (A.6) by $\frac{(f_j, x_0)}{\lambda - \exp(t\nu_j)}$ and summing over j we obtain:

$$a_\lambda = a_\lambda \lambda (1 - e^{2t}) \sum_{j=0}^{N-1} \frac{|(x_0, f_j)|^2}{\lambda - \exp(t\nu_j)}.$$

With condition $a_\lambda \neq 0$ and also (A.5) and (A.6) this relation takes the form:

$$1 = \frac{1 - e^{2t}}{M} \left(\frac{1}{1 - \exp(t\xi)} + \frac{1}{2} \sum_{j=1}^{M-1} \frac{4 + \nu_j}{1 - \exp(t(\nu_j - \xi))} \right), \tag{A.9}$$

where $\xi = \ln \frac{\lambda}{t}$. It is easy to see that equation (A.9) has exactly M real roots, one in each interval (ν_j, ν_{j+1}) , where $j = 0, 1, \dots, M-1$. These roots can be easily found numerically by the bisection method.

Denote the solutions of (A.9) by $\xi_j(t)$, where $j = 1, 2, \dots, M$. Then, for the spectrum $\lambda_j(t)$, where $j = 0, 1, \dots, N-1$, of operator $\hat{S}_2(t)$ we finally obtain:

$$\lambda_{2j}(t) = \exp(t\xi_j(t)), \quad \lambda_{2j+1} = \exp(t\nu_j), \quad j = 0, 1, \dots, M-1.$$

Note that for the eigenvalues $\lambda(t) = \exp(it\xi(t))$ of the step operator $\hat{S}_2(t)$ corresponding to (Schrödinger) operator $i\hat{\Delta}_D$ equation (A.9) is of the form:

$$1 = \frac{\tan t}{M} \left(-\frac{1}{\tan(\frac{1}{2}t\xi)} + \frac{1}{2} \sum_{j=1}^{M-1} \frac{4 + \nu_j}{\tan(\frac{1}{2}t(\nu_j - \xi))} \right).$$

The solutions of this equation are in good agreement with those of (A.9).

Acknowledgements

We are thankful to E I Gordon and M A Antonets for fruitful discussions. The work is partially supported by the RFBR grant 99-02-16188.

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