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AN EFFICIENT NUMERICAL METHOD FOR PARABOLIC EQUATIONS

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Abstract

Parabolic partial differential equations frequently arise in computational physics. For instance, a nonstationary heat equation and diffraction one in a paraxial approach are of this type. A system of ordinary differential equations obtained from the initial one by discretization of the spatial Laplace operator is stiff or has rapidly oscillating parasitic solutions, so an A-stable method is to be used to solve it. All these methods include decomposition of a huge size matrix, so can not be effective. In addition, a conventional three-node numerical formula for the Laplacian provides only second approximation order that is also not effective.

An efficient numerical method for parabolic equations is proposed and investigated. It is based on the second order Rosenbrock method for the independent coordinate with a special procedure of matrix pseudoinversion and a three-node formula with a Numerov's corrector for the spatial Laplacian.

Key words

Parabolic equation, 4^{th} spatial order numerical method, 2^{nd} temporal order A-stable numerical method, Numerov's corrector, implicit pseudoinversion of infinite matrices.

1 Introduction

Parabolic partial differential equations (PPDE) often arise in computational physics. We shall consider here a particular case of PPDE without first spatial derivatives and in a homogeneous space:

$$\frac{\partial}{\partial t}\phi(x,t) = D\Delta\phi(x,t) + f(x,t), \qquad (1)$$

where ϕ, x, and f can be scalars or vectors. Note that D can be real, as in the heat equation or imaginary as in the paraxial diffraction one. If one discretizes the right part by x using, say, a conventional three-node formula, then he obtains a set of ordinary differential equations (SODE) to be solved using some numerical method along t. The problem is that the SODE obtained is stiff (if D is real) or has rapidly oscillating parasitic solutions (if D is imaginary; also usually called "stiff"). Let us demonstrate it. Consider a unidimensional scalar PPDE:

$$\frac{\partial}{\partial t}\phi(x,t) = D\frac{\partial^2}{\partial x^2}\phi(x,t) + f(x,t).$$

Taking a uniform spatial grid of a step Δ and applying a three-node approximation formula for the Laplace op-

erator

$$\frac{\partial^2}{\partial x^2}\phi(x) \sim \frac{\phi(x+\Delta x)+\phi(x-\Delta x)-2\phi(x)}{(\Delta x)^2}, \quad (2)$$

one obtains a SODE:

$$\frac{\partial}{\partial t}\phi(x_j,t) = D\frac{\phi(x_{j+1})+\phi(x_{j-1})-2\phi(x_j)}{(\Delta x)^2} + f(x_j,t),$$

where j is the node index. The corresponding homogeneous SODE

$$\frac{\partial}{\partial t}\phi(x_j,t) = D\frac{\phi(x_{j+1})+\phi(x_{j-1})-2\phi(x_j)}{(\Delta x)^2} \quad (3)$$

has the following full set of solutions:

$$\phi(x_j,t) = Aexp(ikx+\lambda t),$$

where A is an arbitrary amplitude, i is the imaginary unit, and

$$\lambda = \frac{2D}{(\Delta x)^2}\left(cos(k\Delta x)-1\right), 0 \le |k| \le \frac{\pi}{\Delta x}.$$

Thus, λ varies from 0 to $-4D/(\Delta x)^2$. If one would like to improve accuracy and decrease Δx, the minimum λ/D ratio tends to minus infinity. We do not need these rapidly decreasing (if D is real) or oscillating (if D is imaginary) solutions, but they exist and destroy the stability of conventional numerical methods. It forces to decrease the integration step $\propto \Delta x^2$ and makes the procedure very ineffective [Hairer and Wanner, 1996]. One can use a dedicated method for stiff equations, but all of them need to calculate a Jacobian matrix, then some other matrix specific for the method and to invert it. Of course, the inversion is never executed explicitly. LU decomposition is used instead. Although the initial matrix for n dimensions is sparse (the number of off-diagonal elements in each row is proportional to n) and corresponds to an n-dimensional graph, its filling increases dramatically during the decomposition process, so the cost is unacceptably high for any significant spatial grid size. The necessary number of operations is proportional to $N^{3/2}$ in 2D- and N^2 in 3D-space, where N is the number of nodes in the spatial grid, [Pissanetzky, 1984] Table 4.1. Another significant note is that if D is pure imaginary, the method is to be stable in the whole left complex half-plane of the eigenvalues of the SODE, so no A(α)-stable multistep method can be applied in this case.

2 Numerical Method

As there is no effective numerical method for the general case, ones for particular cases should be developed. The basic idea is to avoid extremely expensive explicit LU decomposition of a huge matrix claimed by all A- or A(α)-stable numerical methods for SODE.

2.1 Basic Method

First of all, consider a simplest numerical method for the two-dimensional equation (1)

$$\left[\frac{\partial}{\partial t} - D\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\right]\phi(x,y,t) = f(x,y,t). \quad (4)$$

Generate a regular rectangular grid with steps Δx and Δy for x and y respectively, consider function values in its nodes only, and replace the initial Laplacian by the numerical one

$$\left[\frac{d}{dt} - D\left(\frac{\mathbf{A}_x}{\Delta x^2}+\frac{\mathbf{A}_y}{\Delta y^2}\right)\right]\vec{\phi}(t) = \mathbf{f}(t), \quad (5)$$

where $\vec{\phi}$ and $\mathbf{f}$ are vectors, while $\mathbf{A}_x$ and $\mathbf{A}_y$ are basis matrices of the numerical Laplacian. The forms of the matrices depend on the method of numeration of nodes in the grid. All their diagonal elements are -2, and they have not more than two off-diagonal elements $A_{jl}=1$, where j and l are the numbers of neighbours by x and y respectively. For example, if one numbers nodes consequently within each raw (y = const) and then rows (also consequently), $\mathbf{A}_x$ will be tridiagonal. Each $\mathbf{A}_x$ and $\mathbf{A}_y$ can be reduced to the tridiagonal form by simultaneous permutation of rows and columns (that is renumbering of grid nodes), but not simultaneously. Both are always sparse.

Next choose a step τ for t and apply an A-stable one-stage Rosenbrock method of the second order [Rosenbrock, 1963]

$$\vec{\phi}(t+\tau) = \vec{\phi}(t) + \tau\left(\mathbf{I} - \frac{\tau}{2}D\left(\frac{\mathbf{A}_x}{\Delta x^2}+\frac{\mathbf{A}_y}{\Delta y^2}\right)\right)^{-1} \times D\left(\frac{\mathbf{A}_x}{\Delta x^2}+\frac{\mathbf{A}_y}{\Delta y^2}\right)\vec{\phi}(t) + \tau\mathbf{f}(t+\tau/2). \quad (6)$$

The term $\mathbf{f}(t)$ not depending on x and y does not affect the stability, so it is not necessary to include it to the Rosenbrock method explicitly. Now one needs to factorize

$$\left(\mathbf{I} - \frac{\tau}{2}D\left(\frac{\mathbf{A}_x}{\Delta x^2}+\frac{\mathbf{A}_y}{\Delta y^2}\right)\right)$$

to make a step by this method. Although the matrix is sparse, it corresponds to a flat graph, and the procedure seems to be very expensive. Let us try to find a

more effective way to solve Eq. (6). Decompose the Rosenbrock corrector into two parts:

$$\vec{\phi}(t+\tau) = \vec{\phi}(t) + \tau \left(\mathbf{I} - \frac{\tau}{2} D \frac{\mathbf{A}_x}{\Delta x^2}\right)^{-1} \times \left(\mathbf{I} - \frac{\tau}{2} D \frac{\mathbf{A}_y}{\Delta y^2}\right)^{-1} D \left(\frac{\mathbf{A}_x}{\Delta x^2} + \frac{\mathbf{A}_y}{\Delta y^2}\right) \vec{\phi}(t) + \tau \mathbf{f}(t+\tau/2). \quad (7)$$

This equation differs from Eq. (6), so check its stability properties first. $\mathbf{f}(t)$ does not affect stability, so we should analyze a homogeneous equation

$$\vec{\phi}(t+\tau) = \vec{\phi}(t) + \tau \left(\mathbf{I} - \frac{\tau}{2} D \frac{\mathbf{A}_x}{\Delta x^2}\right)^{-1} \times \left(\mathbf{I} - \frac{\tau}{2} D \frac{\mathbf{A}_y}{\Delta y^2}\right)^{-1} D \left(\frac{\mathbf{A}_x}{\Delta x^2} + \frac{\mathbf{A}_y}{\Delta y^2}\right) \vec{\phi}(t). \quad (8)$$

Regard the grid as infinite by both coordinates. Consider a spatial harmonics $(k_x)^j (k_y)^l$, where $|k_x| = |k_y| = 1$, while j and l are the indices of nodes by x and y respectively. Then a step (8) is equivalent to multiplication of $\vec{\phi}$ by

$$\alpha = 1 + D\tau \frac{(k_x-1)^2/(k_x\Delta x^2) + (k_y-1)^2/(k_y\Delta y^2)}{(1 - D\tau(k_x-1)^2/2(k_x\Delta x^2))} \to \frac{}{(1 - D\tau(k_y-1)^2/2(k_y\Delta y^2))} = \frac{(1-D_x)(1-D_y)}{(1+D_x)(1+D_y}, \quad (9)$$

where $D_\zeta = D\tau(1 - \mathrm{Re}k_\zeta)/(\Delta\zeta)^2$, and ζ is x or y. Then

$$|\alpha| = \left|\frac{(1-D_x)}{(1+D_x)}\right| \cdot \left|\frac{(1-D_y)}{(1+D_y)}\right|.$$

Note that the expression consists of two multipliers depending on k_x and Δx or k_y and Δy only, so we can analyze them separately and similarly.

$$\left|\frac{(1-D_x)}{(1+D_x)}\right| = \frac{\sqrt{\xi^2 - \xi + \eta^2 + 1}}{\sqrt{\xi^2 + \xi + \eta^2 + 1}},$$

where $\xi = \mathrm{Re}D_x$ and $\eta = \mathrm{Im}D_x$. $\xi \geq 0$, otherwise the initial equation (4) has infinitely increasing solutions, so is unstable itself. In this case

$$\xi^2 + \xi + \eta^2 + 1 \geq \xi^2 - \xi + \eta^2 + 1.$$

Thus $|\alpha| \leq 1$ and the modified method (7) is A-stable.

Let us check the approximation order of Eq. (7). The Rosenbrock corrector in Eq. (6) can be written in the following form:

$$\left(\mathbf{I} - \frac{\tau}{2}(\mathbf{J}_x + \mathbf{J}_y)\right)^{-1},$$

where $\mathbf{J}_\zeta = D\mathbf{A}_\zeta/\Delta\zeta^2$are the Jacobian matrices of the split right part. We need further two properties of $\mathbf{J}_\zeta$. First one is that they have equal eigenvectors $(k_x)^j (k_y)^l$, where $|k_x| = |k_y| = 1$ (corresponding to the eigenvalues $D(k_\zeta + k_\zeta^{-1} - 2)/\Delta\zeta^2$), and this set is a basis. This statement is trivial and can be easily verified by substitution. Second one is commutativity $\mathbf{J}_x\mathbf{J}_y = \mathbf{J}_y\mathbf{J}_x$. Let us prove it. Note first that the coordinates x and y are absolutely similar and the difference between $\mathbf{A}_x$ and$\mathbf{A}_y$ is due to the numeration way of the spatial grid. Thus $\mathbf{A}_y$ can be obtained from $\mathbf{A}_x$ by appropriate renumbering of nodes or, in other words, by a number of simultaneous permutations of rows and columns of equal numbers:

$$\mathbf{J}_y = \mathbf{P}_M \cdots \mathbf{P}_1 \cdot \mathbf{A}_x \cdot \mathbf{P}_1 \cdots \mathbf{P}_M,$$

where $\mathbf{P}_j$ are elementary permutation matrices that is identity matrices with two permutated rows (or columns, this is equal), $\mathbf{P}^T = \mathbf{P}_j^{-1} = \mathbf{P}_j$. Then

$$\begin{aligned}\mathbf{A}_x\mathbf{A}_y &= \mathbf{A}_x \cdot \mathbf{P}_M \cdots \mathbf{P}_1 \cdot \mathbf{A}_x \cdot \mathbf{P}_1 \cdots \mathbf{P}_M \\ &= \left(\mathbf{P}_M^T \cdots \mathbf{P}_1^T \cdot \mathbf{A}_x^T \cdot \mathbf{P}_1^T \cdots \mathbf{P}_M^T \cdot \mathbf{A}_x^T\right)^T \\ &= \mathbf{A}_y\mathbf{A}_x,\end{aligned}$$

as $\mathbf{A}_\zeta$ and $\mathbf{P}_j$ are symmetric. Hence $\mathbf{J}_x$ and $\mathbf{J}_y$ are also commutative. Then

$$\begin{aligned}&\left(\mathbf{I} - \frac{\tau}{2}(\mathbf{J}_x + \mathbf{J}_y)\right)^{-1} \\ &= \left(\left(\mathbf{I} - \frac{\tau}{2}\mathbf{J}_x\right)\left(\mathbf{I} - \frac{\tau}{2}\mathbf{J}_y\right) - \frac{\tau^2}{4}\mathbf{J}_x\mathbf{J}_y\right)^{-1} \\ &= \left(\mathbf{I} - \frac{\tau}{2}\mathbf{J}_y\right)^{-1}\left(\mathbf{I} - \frac{\tau}{2}\mathbf{J}_x\right)^{-1} + O\left(\tau^2\right),\end{aligned}$$

Thus the neglected term has the order τ^3 (together with combined with the right part in Eq. (6)) and does not affect the approximation order. If $\mathbf{J}_x$ and $\mathbf{J}_y$ have eigenvalues g_x and g_y (see above) for some common eigenvector than the residual term of the method is $\tau^3(g_x^3 + g_y^3)/12$.

2.2 Factorization of infinite matrices

Suppose that the Rosenbrock matrices $\mathbf{I} - \tau\mathbf{J}_\zeta/2$ in Eq. (7) are infinite, or, in other words, the area in xy-plane is infinite. Suppose also the spatial grid is numerated in such a way that $\mathbf{J}_\zeta$ is tridiagonal. Let us apply

Gaussian elimination by rows top-down to the each of them. If the initial matrix is

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdots & 0 & b & a & b & 0 & 0 & \cdots \\ \cdots & 0 & 0 & b & a & b & 0 & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

then the stationary state after elimination of some part of upper rows is

$$\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdots & 0 & c & b & 0 & 0 & \cdots \\ \cdots & 0 & b & a & b & 0 & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

where the third row is to be eliminated in the current step. The condition

$$a - b^2/c = c$$

is equivalent to the process stationarity. This equation has two solutions

$$c = \frac{1}{2}\left(a \pm \sqrt{a^2 - 4b^2}\right)$$

and only one with "+" sign gives a stable process. In our case

$$a = 1 + \frac{\tau D}{\Delta\zeta^2}, b = -\frac{\tau D}{2\Delta\zeta^2}$$

Thus we LU decomposed an infinite matrix $(\mathbf{I} - \tau\mathbf{J}_\zeta/2)$:

$$\mathbf{L} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdots & 0 & b/c & 1 & 0 & 0 & \cdots \\ \cdots & 0 & 0 & b/c & 1 & 0 & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

$$\mathbf{U} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdots & 0 & c & b & 0 & 0 & \cdots \\ \cdots & 0 & 0 & c & b & 0 & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}.$$

Now we do not need to factorize the matrix in Eq. (6) explicitly. Instead, we only are to apply back-substitution with known coefficients, namely the following procedure for x and y coordinates consequently:

$$1^0.\ \phi_j \leftarrow \phi_j/c; j = 1...N,$$
$$2^0.\ \phi_{j+1} \leftarrow \phi_{j+1} - b\phi_j; j = 1...N,$$
$$3^0.\ \phi_j \leftarrow \phi_j - b/c\phi_j; j = N...1,$$

where ϕ_j and ϕ_{j+1} mean the function values in the neighboring nodes spaced by Δx or Δy. "$\leftarrow$" means "set the value to the memory cell". The procedure is applied to each line of the grid by x and y independently. Steps 1^o and 2^o are executed in one direction, while 3^o in the opposite. The order of $x-$ and $y-$stages does not affect the result due to commutativity of the partial matrices.

In the long run, we obtained an algorithm of N computational complexity, where N is the number of nodes in the grid. The method can be easily extended to any spatial dimension, and the time complexity remains N. It is worth to remind, for comparison, that the most effective algorithms for sparse matrices have the factorization computational complexities $N^{3/2}$ for 2D grids, N^2 for 3D ones, etc. ([Pissanetzky, 1984] Table 4.1). Note that boundary conditions can not be applied reasonably in this algorithm, as even a huge finite matrix being factorized differs from infinite one near the edges of the spatial grid.

2.3 Boost of the approximation order

The approximation order of the obtained algorithm is two that seems to be not so good. Let us try to improve this feature using the Numerov's formula [Hairer, Norsett, and Wanner, 1993] Chapter III (10.8)

$$\frac{1}{12}\phi^{"}(x - \Delta x) + \frac{5}{6}\phi^{"}(x) + \frac{1}{12}\phi^{"}(x + \Delta x) \sim \frac{\phi(x - \Delta x) - 2\phi(x) + \phi(x + \Delta x)}{\Delta x^2}. \quad (10)$$

The formula permits to calculate the second derivative of a function and has the fourth approximation order. Its drawback is that it is implicit. In our case this drawback does not matter at all, as substitution of Eq. (10) instead of Eq. (2) into Eq. (4) means change in the matrices coefficients in Eq. (7) only.

Let us define two Numerov's matrices $\mathbf{A}_x^N$ and $\mathbf{A}_y^N$ similar to $\mathbf{A}_x$ and $\mathbf{A}_y$ above: all their diagonal elements are 5/6, and they have not more than two off-diagonal elements $A_{jl} = 1/12$, where j and l are the numbers of neighbours by x and y respectively. Then a forth order approximation of the second derivative is

$$\frac{\partial^2\phi}{\partial\zeta^2} \sim \left(\mathbf{A}_\zeta^N\right)^{-1} \frac{\mathbf{A}_\zeta}{\Delta\zeta^2}\vec{\phi}.$$

Substituting this equation into Eq. (4) one obtains

$$\left[\frac{d}{dt} - D\left(\left(\mathbf{A}_x^N\right)^{-1} \frac{\mathbf{A}_x}{\Delta x^2} + \left(\mathbf{A}_y^N\right)^{-1} \frac{\mathbf{A}_y}{\Delta y^2}\right)\right]\vec{\phi}(t) = \mathbf{f}(t)$$

instead of Eq. (5). The Rosenbrock method transforms

it into

$$\vec{\phi}(t+\tau) = \vec{\phi}(t) + \tau\left(\mathbf{I} - \frac{\tau}{2}D\left(\left(\mathbf{A}_x^N\right)^{-1}\frac{\mathbf{A}_x}{\Delta x^2} + \left(\mathbf{A}_y^N\right)^{-1}\frac{\mathbf{A}_y}{\Delta y^2}\right)\right)^{-1} \times \left(\left(\mathbf{A}_x^N\right)^{-1}\frac{\mathbf{A}_x}{\Delta x^2} + \left(\mathbf{A}_y^N\right)^{-1}\frac{\mathbf{A}_y}{\Delta y^2}\right)\vec{\phi}(t) + \tau\mathbf{f}(t+\tau/2)$$

and further

$$\vec{\phi}(t+\tau) = \vec{\phi}(t)\tau\left(\mathbf{I} - \frac{\tau}{2}D\left(\mathbf{A}_x^N\right)^{-1}\frac{\mathbf{A}_x}{\Delta x^2}\right)^{-1} \times \left(\mathbf{I} - \frac{\tau}{2}D\left(\mathbf{A}_y^N\right)^{-1}\frac{\mathbf{A}_y}{\Delta y^2}\right)^{-1} \times D\left(\frac{\tau}{2}D\left(\left(\mathbf{A}_x^N\right)^{-1}\frac{\mathbf{A}_x}{\Delta x^2} + \left(\mathbf{A}_y^N\right)^{-1}\frac{\mathbf{A}_y}{\Delta y^2}\right)\right)\vec{\phi}(t) + \tau\mathbf{f}(t+\tau/2) = \vec{\phi}(t) + \tau\left(\mathbf{A}_x^N - \frac{\tau}{2}D\frac{\mathbf{A}_x}{\Delta x^2}\right)^{-1}\left(\mathbf{A}_y^N - \frac{\tau}{2}D\frac{\mathbf{A}_y}{\Delta y^2}\right)^{-1} \times D\left(\mathbf{A}_y^N\frac{\mathbf{A}_x}{\Delta x^2} + \mathbf{A}_x^N\frac{\mathbf{A}_y}{\Delta y^2}\right)\vec{\phi}(t) + \tau\mathbf{f}(t+\tau/2)$$

after decomposition. Properties $\mathbf{A}_\zeta^N\mathbf{A}_\psi = \mathbf{A}_\psi\mathbf{A}_\zeta^N$, where ζ and ψ mean x or y, and $\mathbf{AB} = \mathbf{BA} \Rightarrow \mathbf{AB}^{-1} = \mathbf{B}^{-1}\mathbf{A}$ were used above. The coefficients in the matrices to be decomposed are now

$$a = \frac{5}{6} + \frac{\tau D}{\Delta\zeta^2}, b = \frac{1}{12} - \frac{\tau D}{2\Delta\zeta^2}.$$

Also two additional products by $\mathbf{A}_x^N$ and $\mathbf{A}_y^N$ are to be calculated in the new method.

In comparison with Eq. (7), we only improved the approximation order for spatial coordinates, so we do not need to check those of the whole method once more. However, we should analyze its stability properties. Let us make a similar formula manipulation as Eq. (7) $\rightarrow$ Eq. (9).

$$\alpha = 1 + \frac{D\tau}{12} \times \frac{(k_y^2+10k_y+1)(k_x-1)^2/(k_xk_y\Delta x^2)}{\left(\frac{(k_x^2+10k_x+1)}{12k_x} - \frac{D\tau(k_x-1)^2}{(2k_x\Delta x^2)}\right)} \rightarrow \frac{+(k_x^2+10k_x+1)(k_y-1)^2/(k_xk_y\Delta y^2)}{\left(\frac{(k_y^2+10k_y+1)}{12k_y} - \frac{D\tau(k_y-1)^2}{(2k_y\Delta y^2)}\right)} = \frac{(N_x-D_x)(N_y-D_y)}{(N_x+D_x)(N_y+D_y)},$$

where D_ζ were defined above, and $N_\zeta = 5/6 + 1/6\mathrm{Re}k_\zeta$. Substituting $d_\zeta = D_\zeta/N_\zeta$ we find

$$|\alpha| = \left|\frac{(1-d_x}{1+d_x}\cdot\frac{1-d_y}{1+d_y}\right|.$$

$\mathrm{Re}d_\zeta \geq 0$ for the same reason as $\mathrm{Re}D_\zeta \geq 0$, so the new method is also A-stable.

3 Numerical Test

Let us use the well-known equation for paraxial wave propagation [Levy, 2000] Eq. (2.21)

$$\left[2ik\frac{\partial}{\partial z} + \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\right]u = 0 \qquad (11)$$

in free space without sources. z is the independent coordinate here (as t previously), and k is the wavenumber. This equation has an analytical solution for the fundamental Gaussian mode, so we can easily evaluate the accuracy. The exact solution is

$$|u| = u_o\frac{w_o}{w}\exp(-r^2/w^2),$$

where u_o is the initial amplitude at the axis, w_o is the initial size, $r^2 = x^2 + y^2$, and

$$w^2 = w_o^2\left[1 + \left(\frac{2z}{kw_o^2}\right)^2\right].$$

The radius of curvature of the wavefront is

$$R = z\left[1 + \left(\frac{kw_o^2}{2z}\right)^2\right].$$

One should multiply $|u|$ by the phase factor

$$\exp\left(i\frac{kr^2}{2R}\right)$$

to obtain the full complex amplitude. In the one-dimensional case, the equation is

$$\left(2ik\frac{\partial}{\partial z} + \frac{\partial^2}{\partial x^2}\right)u = 0, \qquad (12)$$

and its exact solution is

$$|u| = u_o\sqrt{\frac{w}{w_o}}\exp(-x^2/w^2).$$

The phase factor is

$$\exp\left(i\frac{kx^2}{2R}\right)$$

Table 1. Relative accuracy of the basic method

Nodes per grid half-size	Steps by z	$\lvert\Delta u/u\rvert$
One dimension		
60	32	8×10^{-4}
60	25	8.3×10^{-4}
60	16	1×10^{-3}
60	8	2×10^{-3}
60	4	6×10^{-3}
60	2	1.8×10^{-2}
60	1	4.6×10^{-2}
15	32	1.1×10^{-2}
30	32	3×10^{-3}
120	32	2.5×10^{-4}
Two dimensions		
60	32	1×10^{-3}
60	16	1.2×10^{-3}
60	8	1.9×10^{-3}
42	32	2×10^{-3}
30	32	4×10^{-3}
15	8	1.7×10^{-2}
84	32	5.6×10^{-4}

Table 2. Relative accuracy of the improved method

Nodes per grid half-size	Steps by z	$\lvert\Delta u/u\rvert$
60	32	8.8×10^{-5}
30	32	1.2×10^{-4}
15	32	6.5×10^{-4}
8	32	8.3×10^{-3}

Every time numerical simulation was conducted in the interval $z = [0, kw_o^2/2]$, and the initial radius of curvature was $R = \infty$. In this case the final size exceeds the initial one by $\sqrt{2}$ times. The grid half-size was $4.5w_o$, which is quite enough to suppress any significant influence of the edges. The purpose of the numerical test was not detailed investigation of the algorithm properties for various equations, but only a proof of its workability and stability, and an estimation of its accuracy. The results for the basic method and the improved one are collected in Table 1 and Table 2 respectively. Only the 2D problem Eq. (11) results are presented for the improved method.

It is clear from Table 1 that the basic method is stable for all the reasonable ratios $\Delta z/\Delta x$. For example, $\Delta z/k\Delta x^2 \approx 90$ for one step by z and 60 nodes per grid half-size, and the method still gives quite reasonable solution in this case. For reference, the Euler method applied to Eq. (12) $\rightarrow$ (3) is unstable for any $\Delta z/k\Delta x^2$, as in this case

$$\max|\alpha| = |1 + 2ik\Delta z/k\Delta x^2| > 1.$$

For the most well-known Kutta method [Hairer, Nosett, and Wanner, 1993] Chapter II Table 1.2

$$|\alpha| = \frac{1}{24}\sqrt{\vartheta^8\left(\frac{\Delta z}{k\Delta x^2}\right)^8 - 8\vartheta^6\left(\frac{\Delta z}{k\Delta x^2}\right)^6 + 576},$$

where $\vartheta \in [0, 2]$. In this case $\max|\alpha| > 1$ if $\Delta z/k\Delta x^2 > \sqrt{2}$.

The dependence of the relative accuracy of the basic method on the number of steps is shown in Fig. 1. The data from Table 1 were used. One can see the error decreases a little slower than the number of steps to the minus second power. It means the "practical" approximation order in this case is a little less than two. The

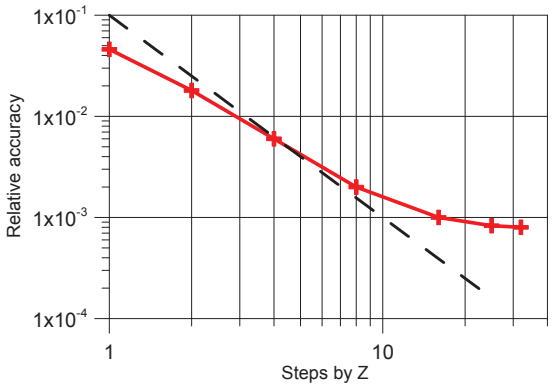

Figure 1. Basic method accuracy vs number of integration steps (solid). $0.1/N^2$ (dashed)

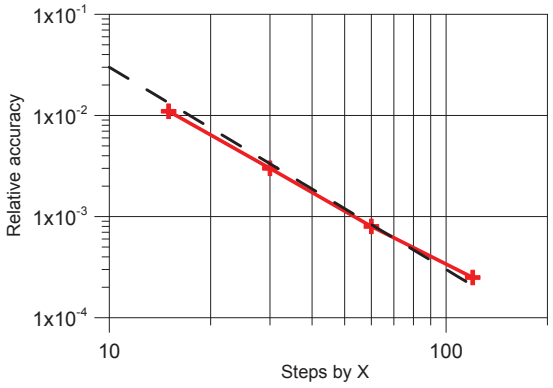

Figure 2. Basic method accuracy vs number of nodes per grid half-size (solid). $3/N^2$ (dashed)

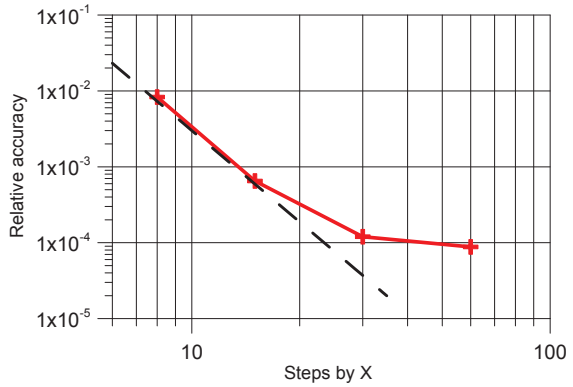

Figure 3. Improved method accuracy vs number of nodes per grid half-size (solid). $30/N^4$ (dashed)

dependence of the accuracy on the number of nodes is represented in Fig. 2. The "practical" approximation order here is exactly two.

The results for the improved method are placed in Fig. 3. One can see that the "practical" approximation for xy is four and the accuracy is limited by Δz. The improved method is obviously better than the basic one as the grid size necessary for some reasonable accuracy is much smaller in this case. Some more details one can find in [Miginsky, 2011].

4 Discussion and Conclusions

Thus we obtained an effective numerical method for parabolic partial differential equations of arbitrary dimension and no boundary condition. Its spatial approximation order is four and the temporal one is two, while its computational complexity is the number of spatial nodes. It is stable for arbitrary ratio of spatial and temporal steps. The method has been numerically tested, and the tests proved its operability, approximation order, and stability.

The spatial approximation order can be enhanced using, say, five-node numerical Laplacian approximation with a Numerov-like corrector. Hardly it makes any practical sense. The temporal order can be raised using a higher order Rosenbrock method. In this case the right part $\mathbf{f}(t)$ not depending on $\vec{\phi}$ should be integrated over a step using a higher-order quadrature, say, Simpson's one having the 4th order. Boundary conditions can be introduced for some price: it is necessary to decompose once the appropriate (split) matrices for each spatial coordinate and keep their elements.

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