Chapter 7
The Diffusion Equation

The diffusion equation is a partial differential equation which describes density fluctuations in a material undergoing diffusion. The equation can be written as:

$$\frac{\partial u(\mathbf{r},t)}{\partial t} = \nabla \cdot \big(D(u(\mathbf{r},t),r)\nabla u(\mathbf{r},t)\big)\,, \tag{7.1}$$

where $u(\mathbf{r},t)$ is the density of the diffusing material at location $\mathbf{r} = (x,y,z)$ and time t. $D(u(\mathbf{r},t),r)$ denotes the collective *diffusion coefficient* for density u at location $\mathbf{r}$. If the diffusion coefficient doesn't depend on the density, i.e., D is constant, then Eq. (7.1) reduces to the following linear equation:

$$\frac{\partial u(\mathbf{r},t)}{\partial t} = D\nabla^2 u(\mathbf{r},t)\,. \tag{7.2}$$

Equation (7.2) is also called *the heat equation* and also describes the distribution of a heat in a given region over time.

Equation (7.2) can be derived in a straightforward way from the *continuity equation*, which states that a change in density in any part of the system is due to inflow and outflow of material into and out of that part of the system. Effectively, no material is created or destroyed:

$$\frac{\partial u}{\partial t} + \nabla \cdot \Gamma = 0\,,$$

where Γ is the flux of the diffusing material. Equation (7.2) can be obtained easily from the last equation when combined with the phenomenological Fick's first law, which assumes that the flux of the diffusing material in any part of the system is proportional to the local density gradient:

$$\Gamma = -D\nabla u(\mathbf{r},t)\,.$$

7.1 The Diffusion Equation in 1D

Consider an IVP for the diffusion equation in one dimension:

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2} \tag{7.3}$$

on the interval $x \in [0, L]$ with initial condition

$$u(x, 0) = f(x), \qquad \forall x \in [0, L] \tag{7.4}$$

and Dirichlet boundary conditions

$$u(0, t) = u(L, t) = 0 \qquad \forall t > 0\,. \tag{7.5}$$

7.1.1 Analytical Solution

Let us attempt to find a nontrivial solution of (7.3) satisfying the boundary conditions (7.5) using separation of variables [4], i.e.,

$$u(x,t) = X(x)T(t)\,.$$

Substituting u back into Eq. (7.3) one obtains:

$$\frac{1}{D}\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)}\,.$$

Since the right hand side depends only on x and the left hand side only on t, both sides are equal to some constant value $-\lambda$ ($-$ sign is taken for convenience reasons). Hence, one can rewrite the last equation as a system of two ODE's:

$$X''(x) + \lambda X(x) = 0, \tag{7.6}$$

$$T'(t) + D\lambda T(t) = 0. \tag{7.7}$$

Let us consider the first equation for $X(x)$. Taking into account the boundary conditions (7.5) one obtains ($T(t) \neq 0$ as we are loocking for nontrivial solutions)

$$u(0,t) = X(0)T(t) = 0 \Rightarrow X(0) = 0\,,$$
$$u(L,t) = X(L)T(t) = 0 \Rightarrow X(L) = 0\,.$$

That is, the problem of finding of the solution of (7.3) reduces to the solving of linear ODE and consideration of three different cases with respect to the sign of λ:

1. $\lambda < 0$:

$$X(x) = C_1\, e^{\sqrt{-\lambda}x} + C_2\, e^{-\sqrt{-\lambda}x}\,.$$

Taking into account the boundary conditions one gets $C_1 = C_2 = 0$, so for $\lambda < 0$ only the trivial solution exists.

2. $\lambda = 0$:
$$X(x) = C_1 x + C_2$$
Again, due to the boundary conditions, one gets only trivial solution of the problem ($C_1 = C_2 = 0$).
3. $\lambda > 0$:
$$X(x) = C_1 \cos(\sqrt{\lambda} x) + C_2 \sin(\sqrt{\lambda} x) .$$
Substituting of the boundary conditions leads to the following equations for the constants C_1 and C_2:
$$\begin{aligned} &X(0) = C_1 = 0 , \\ &X(L) = C_2 \sin(\sqrt{\lambda} L) = 0 \Rightarrow \sin(\sqrt{\lambda} L) = 0 \Rightarrow \lambda_n = \left(\frac{\pi n}{L}\right)^2, \quad n = 1, 2, \ldots . \end{aligned}$$
Hence,
$$X(t) = C_n \sin\left(\frac{\pi n}{L} x\right) .$$

That is, the second equation for the function $T(t)$ takes the form:
$$T'(t) + D\left(\frac{\pi n}{L}\right) T(t) = 0 \Rightarrow T(t) = B_n \exp\left(-D\left(\frac{\pi n}{L}\right)^2 t\right),$$
where B_n is constant.

Altogether, the general solution of the problem (7.3) can be written as
$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(\frac{\pi n}{L} x\right) \exp\left(-D\left(\frac{\pi n}{L}\right)^2 t\right), \quad A_n = \text{const} .$$
In order to find A_n one can use the initial condition (7.4). Indeed, if we write the function $f(x)$ as a Fourier series, we obtain:
$$f(x) = \sum_{n=1}^{\infty} F_n \sin\big(\frac{\pi n}{L} x\big) = \sum_{n=1}^{\infty} A_n \sin\big(\frac{\pi n}{L} x\big) ,$$
$$A_n = F_n = \frac{2}{L} \int_0^L f(\xi) \sin\big(\frac{\pi n}{L} \xi\big)\, d\xi .$$
Hence, the genetal solution of Eq. (7.3) reads:
$$\boxed{u(x,t) = \sum_{n=1}^{\infty} \left(\frac{2}{L} \int_0^L f(\xi) \sin\left(\frac{\pi n}{L} \xi\right) d\xi\right) \sin\left(\frac{\pi n}{L} x\right) \exp\left(-D\big(\frac{\pi n}{L}\big)^2 t\right) .} \quad (7.8)$$

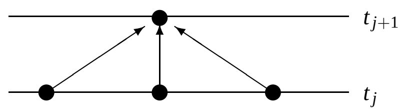

Fig. 7.1 Schematical representation of the FTCS finite difference scheme (7.9) for solving the 1-d diffusion equation (7.3).

7.1.2 Numerical Treatment

The FTCS Explicit Method

Consider Eq. (7.3) with the initial condition (7.4). The first simple idea is an explicit forward in time, central in space (FTCS) method [28, 22] (see Fig. (7.1)):

$$\frac{u_i^{j+1} - u_i^j}{\triangle t} = D\,\frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\triangle x^2}\,,$$

or, with $\alpha = D\frac{\triangle t}{\triangle x^2}$

$$\boxed{u_i^{j+1} = (1 - 2\,\alpha)\,u_i^j + \alpha\,(u_{i+1}^j + u_{i-1}^j)\,.} \tag{7.9}$$

In order to check the stability of the schema (7.9) we apply again the ansatz (1.21) (see Sec. 1.3), considering a single Fourier mode in x space and obtain the following equation for the amplification factor $g(k)$:

$$g^2 = (1 - 2\alpha)g + 2g\alpha\cos(k\triangle x)\,,$$

from which

$$g(k) = 1 - 4\alpha\sin^2\frac{k\triangle x}{2}\,.$$

The stability condition for the method (7.9) reads

$$|g(k)| \le 1 \quad \forall k \Leftrightarrow \alpha \le \frac{1}{2} \Leftrightarrow \boxed{\triangle t \le \frac{1}{2}\frac{\triangle x^2}{D}\,.} \tag{7.10}$$

Although the method (7.9) is conditionally stable, the derived stability condition (7.10), however, hides an uncomfortable property: A doubling of the spatial resolution $\triangle x$ requires a simultaneous reduction in the time-step $\triangle t$ by a factor of four in order to maintain numerical stability. Certainly, the above constraint limits us to absurdly small time-steps in high resolution calculations.

The next point to emphasize is the numerical dispersion. Indeed, let us compare the exact dispersion relation for Eq. (7.3) and relation, obtained by means of the schema (7.9). If we consider the perturbations in form $\exp(ikx - i\omega t)$ the dispersion

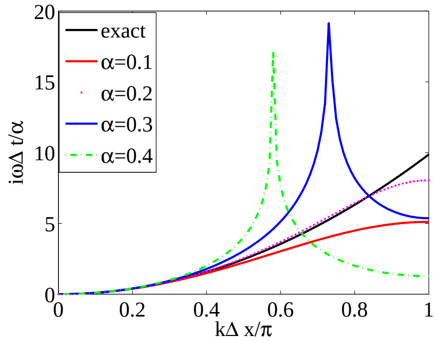

Fig. 7.2 Dispersion relation by means of the schema (7.9) for different values of α, compared with the exact dispersion relation for Eq. (7.3).

relation for Eq. (7.3) reads

$$i\omega = Dk^2\,.$$

On the other hand, the FTCS schema (7.3) leads to the following relation

$$e^{i\omega\triangle t} = 1 - 4\,\alpha\,\sin^2\left(\frac{k\triangle x}{2}\right),$$

or, in other words

$$\boxed{i\omega\triangle t = -\ln\left(1 - 4\alpha\sin^2\left(\frac{k\triangle x}{2}\right)\right)\,.}$$

The comparison between exact and numerical disperion relations is shown on Fig. (7.2). One can see, that both relations are in good agreement only for $k\triangle x \ll 1$. For $\alpha > 0.25$ the method is stable, but the values of ω can be complex, i.e., the Fourier modes drops off, performing damped oscillations (see Fig. (7.2) for $\alpha = 0.3$ and $\alpha = 0.4$). Now, if we try to make the time step smaler, in the limit $\triangle t \to 0$ (or $\alpha \to 0$) we obtain

$$i\omega\triangle t \approx 4\alpha\sin^2\left(\frac{k\triangle x}{2}\right) = k^2 D\triangle t\frac{\sin^2\left(\frac{k\triangle x}{2}\right)}{\left(\frac{k\triangle x}{2}\right)^2}\,,$$

i.e., we get the correct dispersion relation only if the space step $\triangle x$ is small enougth too.

The Richardson Method

The first idea to improve the approximation order of the schema is to use the central diferences for the time derivative of Eq. (7.3), namely [28]

$$\frac{u_i^{j+1}-u_i^{j-1}}{2\triangle t}=D\,\frac{u_{i+1}^j-2u_i^j+u_{i-1}^j}{\triangle x^2}\,,$$

or, with $\alpha=D\triangle t/\triangle x^2$

$$\boxed{u_i^{j+1}=u_i^{j-1}+2\alpha\big(u_{i+1}^j-2u_i^j+u_{i-1}^j\big)\,.} \tag{7.11}$$

Unfortunately, one can show that the schema (7.11) is unconditional unstable. Indeed, amplification factor $g(k)$ in this case fulfilles the following equation:

$$g^2+2\beta g-1=0,\qquad \beta=4\alpha\sin^2\frac{k\triangle x}{2}\,,$$

giving

$$g_{1,2}=-\beta\pm\sqrt{\beta^2+1}\,.$$

Since $|g_2(k)|>1$ for all values of k, the schema (7.11) is absolut unstable.

The DuFort-Frankel Method

Let us consider one of many alternative algorithms which have been designed to overcome the stability problems of the simple FTCS and Richardson methods. We modify Eq. (7.9) as (see Fig. (7.3)) [28]

$$\frac{u_i^{j+1}-u_i^{j-1}}{2\triangle t}=D\,\frac{u_{i+1}^j-2\frac{u_i^{j+1}+u_i^{j-1}}{2}+u_{i-1}^j}{\triangle x^2}\,,$$

which can be solved explicitly for u_i^{j+1}:

$$\boxed{u_i^{j+1}=\frac{1-\alpha}{1+\alpha}u_i^{j-1}+\frac{\alpha}{1+\alpha}\big(u_{i+1}^j+u_{i-1}^j\big)\,,} \tag{7.12}$$

where $\alpha=2D\triangle t/\triangle x$. When the usual von Neumann stability analysis is applied to the method (7.12), the amplification factor $g(k)$ can be found from

$$(1+\alpha)g^2-2g\alpha\cos(k\triangle x)+(\alpha-1)=0\,.$$

It can be easily shown, that stability condition is fulfilled for all values of α, so the method (7.12) is unconditionally stable. However, this does not imply that $\triangle x$ and $\triangle t$ can be made indefinitely large; we must still worry about the accuracy of the

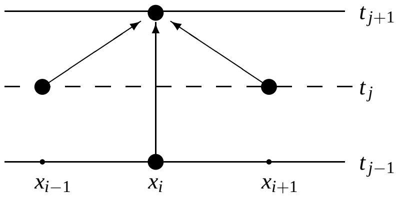

Fig. 7.3 Schematical representation of the DuFort-Frankel method (7.12).

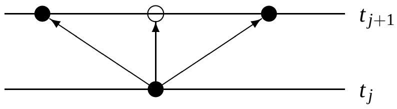

Fig. 7.4 Schematical representation of the implicit BTCS method (7.13).

method. Indeed, consider the Taylor expansion for Eq. (7.3) by means of (7.12):

$$\frac{u_i^{j+1} - u_i^{j-1}}{2\triangle t} = D\frac{u_{i+1}^j - u_i^{j+1} - u_i^{j-1} + u_{i-1}^j}{\triangle x^2} \Leftrightarrow$$

$$u_t - \frac{\triangle x^2}{3!}u_{ttt} + \ldots = \frac{D}{\triangle x^2}\left(\triangle x^2 u_{xx} + \frac{2\triangle x^4}{4!}u_{xxxx} - \triangle t^2 u_{tt} - \frac{2\triangle t^4}{4!}u_{tttt} + \ldots\right) \Leftrightarrow$$

$$u_t + \mathscr{O}(\triangle t^2) = Du_{xx} + \mathscr{O}(\triangle x^2) - D\left(\frac{\triangle t^2}{\triangle x^2}\right)u_{tt} + \mathscr{O}\left(\frac{\triangle t^4}{\triangle x^2}\right).$$

In other words, the method (7.12) has order of accuracy

$$\mathscr{O}\left(\triangle t^2, \triangle x^2, \frac{\triangle t^2}{\triangle x^2}\right).$$

For cosistency, $\triangle t/\triangle x \longrightarrow 0$ as $\triangle t \longrightarrow 0$ and $\triangle x \longrightarrow 0$, so (7.12) is inconsistent. This constitutes an effective restriction on $\triangle t$. For large $\triangle t$, however, the scheme (7.12) is consistent with *another* equation of the form

$$D u_{tt} + u_t = D u_{xx}\,.$$

7.1.2.1 The BTCS Implicit Method

One can try to overcome problems, described above by introducing an implicit method. The simplest example is a BTCS (backward in time, central in space) method (see Fig. 7.4) [29]. The differential schema reads:

$$\frac{u_i^{j+1} - u_i^j}{\triangle t} = D\,\frac{u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}}{\triangle x^2} + \mathscr{O}(\triangle t, \triangle x^2)\,,$$

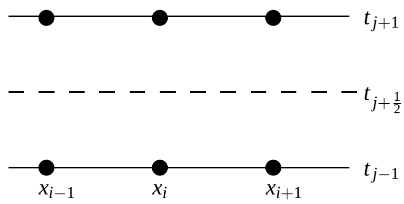

Fig. 7.5 Schematical representation of the Crank-Nicolson method (7.14).

or, with $\alpha = D\triangle t/\triangle x^2$

$$\boxed{-u_i^j = \alpha u_{i+1}^{j+1} - (1+2\alpha)u_i^{j+1} + \alpha u_{i-1}^{j+1}\,.} \tag{7.13}$$

In this case the amplification factor $g(k)$ is given by

$$g(k) = \left(1 + 4\alpha \sin^2 \frac{k\triangle x^2}{2}\right)^{-1}.$$

That is, the schema (7.13) is unconditionally stable. However, the method has order of accuracy $\mathscr{O}(\triangle t, \triangle x^2)$, i.e., first order in time, and second in space. Is it possible to improve it? The answer to is given below.

The Crank-Nicolson Method

An implicit scheme, introduced by J. Crank and P. Nicolson in 1947 [6] is based on the central approximation of Eq. (7.3) at the point $(x_i, t_j + \frac{1}{2}\triangle t)$ (see Fig. (7.5)):

$$\frac{u_i^{j+1} - u_i^j}{2\frac{\triangle t}{2}} = D\,\frac{u_{i+1}^{j+\frac{1}{2}} - 2\,u_i^{j+\frac{1}{2}} + u_{i-1}^{j+\frac{1}{2}}}{\triangle x^2}\,.$$

The approximation used for the space derivative is just an average of approximations in points (x_i, t_j) and (x_i, t_{j+1}):

$$\frac{u_i^{n+1} - u_i^n}{\triangle t} = D\,\frac{(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}) + (u_{i+1}^n - 2u_i^n + u_{i-1}^n)}{2\,\triangle x^2}\,.$$

Introducing $\alpha = D\triangle t/\triangle x^2$ one can rewrite the last equation as

$$\boxed{-\alpha u_{i+1}^{j+1} + 2(1+\alpha)u_i^{j+1} - \alpha u_{i-1}^{j+1} = \alpha u_{j+1}^n + 2(1-\alpha)u_i^j + \alpha u_{j-1}^n\,.} \tag{7.14}$$

All terms on the right-hand side of Eq. (7.14) are known. Hence, the equations in (7.14) form a tridiagonal linear system

$$A\mathbf{u} = \mathbf{b}\,.$$

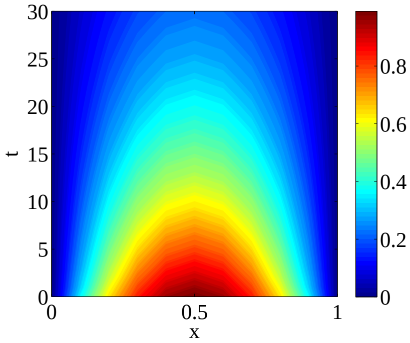

Fig. 7.6 Contour plot of the heat distribution after the time $T = 30$, calculated with the FTCS method (7.9).

The amplification factor for Eq. (7.14) reads

$$g(k) = \frac{1 - \alpha(1 - \cos k\triangle x)}{1 + \alpha(1 - \cos k\triangle x)}.$$

Since α and $1 - \cos k\triangle x$ are positive, the denominator of the last expression is always greater than the numerator. That is, the absolute value of g is less than one, i.e., the method (7.14) is unconditionaly stable.

7.1.3 Examples

Example 1

Use the FTCS explicit method (7.9) to solve the one-dimensional heat equation

$$u_t = u_{xx},$$

on the interval $x \in [0, L]$, if the initial heat distribution is given by $u(x, 0) = f(x)$, and the temperature on both ends of the interval is $u(0,t) = T_l$, $u(L,t) = T_r$. Other parameters are choosen according to the table below:

`Space interval`	$L = 1$
`Amount of space points`	$M = 10$
`Amount of time steps`	$T = 30$
`Boundary conditions`	$T_l = T_r = 0$
`Initial heat distribution`	$f(x) = 4x(1 - x)$

The result of the calculation is shown on Fig 7.6.

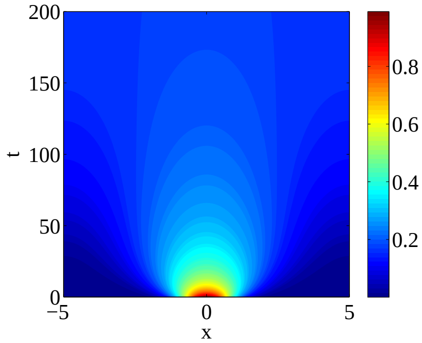

Fig. 7.7 Contour plot of the diffusion of the initial Gauss pulse, calculated with the BTCS implicit method (7.13).

Example 2

Use the implicit BTCS method (7.13) to solve the one-dimensional diffusion equation

$$u_t = u_{xx},$$

on the interval $x \in [-L, L]$, if the initial distribution is a Gauss pulse of the form $u(x,0) = \exp(-x^2)$ and the density on both ends of the interval is given as $u_x(-L,t) = u_x(L,t) = 0$. For the other parameters see the table below:

`Space interval`	$L = 5$
`Space discretization step`	$\triangle x = 0.1$
`Time discretization step`	$\triangle t = 0.05$
`Amount of time steps`	$T = 200$

Solution of the problem is shown on Fig. (7.7).

Example 3

Use the Crank-Nicolson method (7.14) to solve the one-dimensional heat equation

$$u_t = 1.44\, u_{xx},$$

on the interval $x \in [0, L]$, if the initial heat distribution is $u(x,0) = f(x)$ and again, the temperature on both ends of the interval is given as $u(0,t) = T_l$, $u(L,t) = T_r$. Other parameters are choosen as:

`Space interval`	L=1
`Space discretization step`	$\triangle x = 0.1$
`Time discretization step`	$\triangle t = 0.05$
`Amount of time steps`	$T = 15$
`Boundary conditions`	$T_l = 2$, $T_r = 0.5$
`Initial heat distribution`	$f(x) = 2 - 1.5x + \sin(\pi x)$

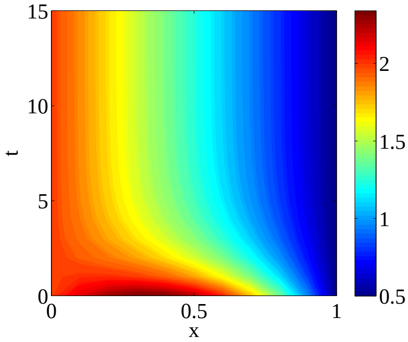

Fig. 7.8 Contour plot of the heat distribution, calculated with the Crank-Nicolson method (7.14).

Numerical solution of the problem in question is shown on Fig. (7.8).

7.2 The Diffusion Equation in 2D

Let us consider the solution of the diffusion equation (7.2) in two dimensions

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{7.15}$$

where $u = u(x,y,t)$, $x \in [a_x, b_x]$, $y \in [a_y, b_y]$. Suppose, that the inittial condition is given and function u satisfies boundary conditions in both x- and in y-directions. As before, we discretize in time on the uniform grid $t_n = t_0 + n\triangle t$, $n = 0, 1, 2, \ldots$. Futhermore, in the both x- and y-directions, we use the uniform grid

$$x_i = x_0 + i\triangle x, \quad i = 0, \cdots, M, \quad \triangle x = \frac{b_x - a_x}{M+1},$$
$$y_j = y_0 + j\triangle y, \quad j = 0, \cdots, N, \quad \triangle y = \frac{b_y - a_y}{N+1}.$$

7.2.1 *Numerical Treatment*

The FTCS Method in 2D

In the case of two dimensions the explicit FTCS scheme reads

$$\frac{u_{ij}^{n+1} - u_{ij}^n}{\triangle t} = D\left(\frac{u_{i+1j}^n - 2u_{ij}^n + u_{i-1j}^n}{\triangle x^2} + \frac{u_{ij+1}^n - 2u_{ij}^n + u_{ij-1}^n}{\triangle y^2}\right),$$

or, with $\alpha = D\triangle t/\triangle x^2$ and $\beta = D\triangle t/\triangle y^2$

$$\boxed{u_{ij}^{n+1} = \alpha(u_{i+1j}^n + u_{i-1j}^n) + \beta(u_{ij+1}^n + u_{ij-1}^n) + (1-2\alpha-2\beta)u_{ij}^n\,.} \tag{7.16}$$

The ansatz

$$\varepsilon_{ij}^n = g^n e^{i(k_x x_i + k_y x_j)}$$

leads to the following relation for the amplification factor $g(k)$

$$g(k) = 1 - 4\alpha\sin^2\left(\frac{k_x\triangle x}{2}\right) - 4\beta\sin^2\left(\frac{k_y\triangle y}{2}\right).$$

In this case the stability condition reads

$$\alpha + \beta \le \frac{1}{2}\,. \tag{7.17}$$

This stability condition imposes a limit on the time step:

$$\boxed{\triangle t \le \frac{\triangle x^2\triangle y^2}{2D(\triangle x^2 + \triangle y^2)}\,.}$$

In particular, for the case $\triangle x = \triangle y$ we have

$$\triangle t \le \frac{\triangle x^2}{4D}\,,$$

which is even more restrictive, than in the one-dimensional case.

The BTCS Method in 2D

To overcome the stability restriction of the FTCS method (7.16), we can use an implicit BTCS schema in the two-dimensional case. The schema reads:

$$\frac{u_{ij}^{n+1} - u_{ij}^n}{\triangle t} = D\left(\frac{u_{i+1j}^{n+1} - 2u_{ij}^{n+1} + u_{i-1j}^{n+1}}{\triangle x^2} + \frac{u_{ij+1}^{n+1} - 2u_{ij}^{n+1} + u_{ij-1}^{n+1}}{\triangle y^2}\right),$$

or

$$\boxed{-\alpha(u_{i+1j}^{n+1} + u_{i-1j}^{n+1}) + (1+2\alpha+2\beta)u_{ij}^{n+1} - \beta(u_{ij+1}^{n+1} + u_{ij-1}^{n+1}) = u_{ij}^n\,.} \tag{7.18}$$

Let us consider the approximation (7.18) on the 5×5 grid, i.e., $i = j = 0,\ldots,4$. Moreover, suppose that Dirichlet boundary conditions are given, that is, all values $u_{0j}, u_{4j}, u_{i0}, u_{i4}$ are known. Suppose also that $n = 1$ and define $\gamma = 1 + 2\alpha + 2\beta$. Then the approximation above leads to the neun algebraic equations:

$$
\begin{aligned}
-\alpha u_{21}^2 + \gamma u_{11}^2 - \beta u_{12}^2 &= u_{11}^1 + \alpha u_{01}^2 + \beta u_{10}^2, \\
-\alpha u_{22}^2 + \gamma u_{12}^2 - \beta (u_{13}^2 + u_{11}^2) &= u_{12}^1 + \alpha u_{02}^2, \\
-\alpha u_{23}^2 + \gamma u_{13}^2 - \beta u_{12}^2 &= u_{13}^1 + \alpha u_{03}^2 + \beta u_{14}^2, \\
-\alpha (u_{31}^2 + u_{11}^2) + \gamma u_{21}^2 - \beta u_{22}^2 &= u_{21}^1 + \beta u_{20}^2, \\
-\alpha (u_{32}^2 + u_{12}^2) + \gamma u_{22}^2 - \beta (u_{23}^2 + u_{21}^2) &= u_{22}^1, \\
-\alpha u_{21}^2 + \gamma u_{31}^2 - \beta u_{32}^2 &= u_{31}^1 + \alpha u_{41}^2 + \beta u_{30}^2, \\
-\alpha u_{22}^2 + \gamma u_{32}^2 - \beta (u_{33}^2 + u_{31}^2) &= u_{32}^1 + \alpha u_{42}^1, \\
-\alpha u_{23}^2 + \gamma u_{33}^2 - \beta u_{32}^2 &= u_{33}^1 + \alpha u_{44}^2 + \beta u_{34}^2.
\end{aligned}
$$

Formally, one can rewrite the system above to the matrix form $A\mathbf{u} = \mathbf{b}$, i.e.,

$$
\left(\begin{array}{ccc|ccc|ccc}
\gamma & -\beta & 0 & -\alpha & 0 & 0 & 0 & 0 & 0 \\
-\beta & \gamma & -\beta & 0 & -\alpha & 0 & 0 & 0 & 0 \\
0 & -\beta & \gamma & 0 & 0 & -\alpha & 0 & 0 & 0 \\
\hline
-\alpha & 0 & 0 & \gamma & -\beta & 0 & -\alpha & 0 & 0 \\
0 & -\alpha & 0 & -\beta & \gamma & -\beta & 0 & -\alpha & 0 \\
0 & 0 & -\alpha & 0 & -\beta & \gamma & 0 & 0 & -\alpha \\
\hline
0 & 0 & 0 & -\alpha & 0 & 0 & \gamma & -\beta & 0 \\
0 & 0 & 0 & 0 & -\alpha & 0 & -\beta & \gamma & -\beta \\
0 & 0 & 0 & 0 & 0 & -\alpha & 0 & -\beta & \gamma
\end{array}\right)
\left(\begin{array}{c}
u_{11}^2 \\ u_{12}^2 \\ u_{13}^2 \\ \hline u_{21}^2 \\ u_{22}^2 \\ u_{23}^2 \\ \hline u_{31}^2 \\ u_{32}^2 \\ u_{33}^2
\end{array}\right)
=
\left(\begin{array}{c}
u_{11}^1 + \alpha u_{01}^2 + \beta u_{10}^2 \\
u_{12}^1 + \alpha u_{02}^2 \\
u_{13}^1 + \alpha u_{03}^2 + \beta u_{14}^2 \\
\hline
u_{21}^1 + \beta u_{20}^2 \\
u_{22}^1 \\
u_{23}^1 + \beta u_{24}^2 \\
\hline
u_{31}^1 + \alpha u_{41}^2 + \beta u_{30}^2 \\
u_{32}^1 + \alpha u_{42}^2 \\
u_{33}^1 + \alpha u_{44}^1 + \beta u_{34}^2
\end{array}\right)
$$

The matrix A is a five-band matrix. Nevertheless, despite of the fact that the schema is absolute stable, two of five bands are desposed so far apart from the main diagonal, that simple $\mathcal{O}(n)$ algorithms like TDMA are difficult or even impossible to apply.

The ADI Method

The idea of the ADI-method (*alternating direction implicit*) is to alternate direction and thus solve two one-dimensional problem at each time step [17]. The first step keeps y-direction fixed:

$$
\frac{u_{ij}^{n+1/2} - u_{ij}^n}{\triangle t/2} = D\left(\frac{u_{i+1j}^{n+1/2} - 2u_{ij}^{n+1/2} + u_{i-1j}^{n+1/2}}{\triangle x^2} + \frac{u_{ij+1}^n - 2u_{ij}^n + u_{ij-1}^n}{\triangle y^2} \right).
$$

In the second step we keep x-direction fixed:

$$
\frac{u_{ij}^{n+1} - u_{ij}^{n+1/2}}{\triangle t/2} = D\left(\frac{u_{i+1j}^{n+1/2} - 2u_{ij}^{n+1/2} + u_{i-1j}^{n+1/2}}{\triangle x^2} + \frac{u_{ij+1}^{n+1} - 2u_{ij}^{n+1} + u_{ij-1}^{n+1}}{\triangle y^2} \right).
$$

Both equations can be written in a triadiagonal form. Define

$$
\alpha = \frac{D\triangle t}{2\triangle x^2}, \qquad \beta = \frac{D\triangle t}{2\triangle y^2}.
$$

Than we get:

$$-\alpha u_{i+1j}^{n+1/2} + (1+2\alpha)u_{ij}^{n+1/2} - \alpha u_{i-1j}^{n+1/2} = \beta u_{ij+1}^{n} + (1-2\beta)u_{ij}^{n} + \beta u_{ij-1}^{n} \qquad (7.19)$$
$$-\beta u_{ij+1}^{n+1} + (1+2\beta)u_{ij}^{n+1} - \beta u_{ij-1}^{n+1} = \alpha u_{i+1j}^{n+1/2} + (1-2\alpha)u_{ij}^{n+1/2} + \alpha u_{i+1j}^{n+1/2}\,.$$

Instead of five-band matrix in BTCS method (7.18), here each time step can be obtained in two sweeps. Each sweep can be done by solving a tridiagonal system of equations. The ADI-method is second order in time and space and is absolute stable [11] (however, the ADI method in 3D is conditional stable only).

7.2.2 Examples

Use the ADI method (7.19) to solve the two-dimensional diffusion equation

$$\partial_t u(\mathbf{r},t) = \triangle u(\mathbf{r},t)\,,$$

where $u = u(\mathbf{r},t)$, $\mathbf{r} \subseteq \mathbb{R}^2$ on the interval $r \in [0,L] \times [0,L]$, if the initial distribution is a Gauss pulse of the form $u(x,0) = \exp(-20\,(x-L/2)^2 - 20\,(y-L/2)^2)$ and the density on both ends of the interval is given as $u_r(0,t) = u_r(L,t) = 0$. Other parameters are choosen according to the table below.

`Space interval`	$L = 1$
`Amount of points`	$M = 100$, $(\triangle x = \triangle y)$
`Time discretization step`	$\triangle t = 0.001$
`Amount of time steps`	$T = 40$

Solution of the problem is shown on Fig. (7.9).

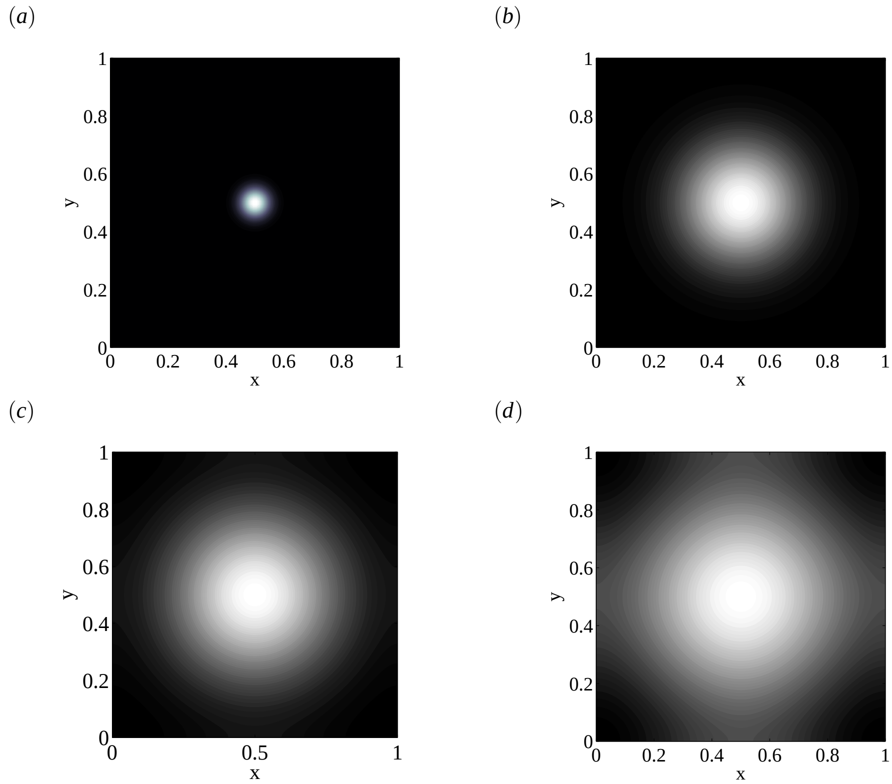

Fig. 7.9 Numerical solution of the two-dimensional diffusion equation 7.2 by means of the ADI method (7.19), calculated at four different time moments: (a) t=0; (b) t=10; (c) t=20; (d) t=40.