Chapter 17
Diffusion

Diffusion is one of the simplest non-equilibrium processes. It describes the transport of heat [90, 91] and the time evolution of differences in substance concentrations [92].

In this chapter we consider the diffusion equation

$$\frac{\partial f}{\partial t} = \mathrm{div}(D \ \mathrm{grad} \ f) + S, \tag{17.1}$$

where D is the diffusion constant (which may depend on position) and S is a source term.

17.1 Basic Physics of Diffusion

Let f denote the concentration of a particle species or the temperature. $\mathbf{J}$ is the corresponding flux of particles. Consider a small cube dx dy dz (Fig. 17.1).

The change of the number of particles within this volume is given by the sum of all incoming and outgoing fluxes

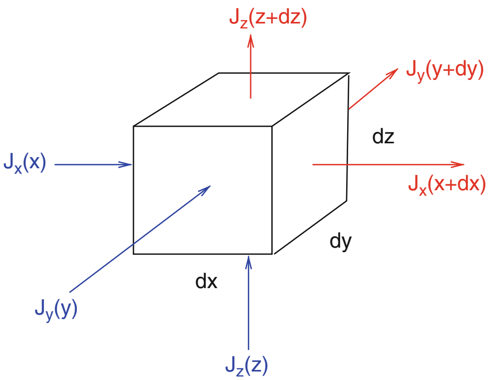

Fig. 17.1 Flux through a volume element dx dy dz

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$$\frac{\partial f}{\partial t}\mathrm{d}x\mathrm{d}y\mathrm{d}z$$
$$= (J_x(x,y,z) - J_x(x+\mathrm{d}x,y,z))\mathrm{d}y\mathrm{d}z \tag{17.2}$$
$$+ (J_y(x,y,z) - J_y(x,y+\mathrm{d}y,z))\mathrm{d}x\mathrm{d}z$$
$$+ (J_z(x,y,z) - J_z(x,y,z+\mathrm{d}z))\mathrm{d}x\mathrm{d}y$$

from which the continuity equation follows:

$$\frac{\partial f}{\partial t} = -\frac{\partial J_x}{\partial x} - \frac{\partial J_y}{\partial y} - \frac{\partial J_z}{\partial z} = -\mathrm{div}\,\mathbf{J}. \tag{17.3}$$

Within the framework of linear response theory the flux is proportional to the gradient of f,

$$\mathbf{J} = -D\ \mathrm{grad}\ f. \tag{17.4}$$

Together we have

$$\mathrm{div}(D\ \mathrm{grad}\ f) = -\mathrm{div}\,\mathbf{J} = \frac{\partial f}{\partial t}. \tag{17.5}$$

Addition of a source (or sink) term completes the diffusion equation. In the special case of constant D it simplifies to

$$\frac{\partial f}{\partial t} = D\Delta f + S. \tag{17.6}$$

17.2 Boundary Conditions

The following choices of boundary conditions are important:

- Dirichlet b.c.: $f(t, x_{\mathrm{bound}})$ given. Can be realized by adding additional points x_{-1} and x_N with given $f(t, x_{-1})$ and $f(t, x_N)$.
- Neumann b.c.: The flux through the boundary is given. Can be realized by adding additional points x_{-1} and x_N with given $f(t, x_{-1}) = f(t, x_0) + D^{-1}\Delta x\ j_1(t)$ and $f(t, x_N) = f(t, x_{N-1}) - D^{-1}\Delta x\ j_{N-1}(t)$.
- No-flow b.c.: no flux through the boundary. Can be realized by a reflection at the boundary. Additional points x_{-1} and x_N are added with $f(t, x_{-1}) = f(t, x_1)$ and $f(t, x_N) = f(t, x_{N-2})$ which compensates the flux through the boundary (Fig. 17.2).

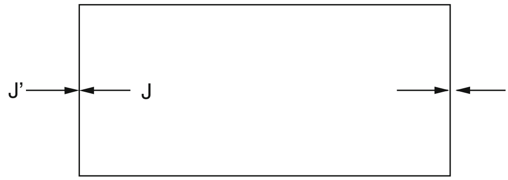

Fig. 17.2 No-flow boundary conditions

17.3 Numerical Integration of the Diffusion Equation

We use discrete values of time and space (one dimensional for now) $t_n = n\Delta t$, $x_m = m\Delta x$, $m = 0, 1, \ldots N-1$ and the discretized derivatives

$$\frac{\partial f}{\partial t} = \frac{f(t_{n+1}, x_m) - f(t_n, x_m)}{\Delta t} \tag{17.7}$$

$$\Delta f = \frac{f(t_n, x_{m+1}) + f(t_n, x_{m-1}) - 2f(t_n, x_m)}{\Delta x^2}. \tag{17.8}$$

17.3.1 Forward Euler or Explicit Richardson Method

A simple Euler step (11.3) is given by

$$f(t_{n+1}, x_m) = f(t_n, x_m) + D\frac{\Delta t}{\Delta x^2}\left(f(t_n, x_{m+1}) + f(t_n, x_{m-1}) - 2f(t_n, x_m)\right) + S(t_n, x_m)\Delta t. \tag{17.9}$$

17.3.2 Stability Analysis

In matrix notation the one-dimensional algorithm with boundary condition $f = 0$ is given by

$$\begin{pmatrix} f(t_{n+1}, x_1) \\ \vdots \\ f(t_{n+1}, x_M) \end{pmatrix} = A \begin{pmatrix} f(t_n, x_1) \\ \vdots \\ f(t_n, x_M) \end{pmatrix} + \begin{pmatrix} S(t_n, x_1)\Delta t \\ \vdots \\ S(t_n, x_M)\Delta t \end{pmatrix} \tag{17.10}$$

with the tridiagonal matrix

$$A = \begin{pmatrix} 1-2D\frac{\Delta t}{\Delta x^2} & D\frac{\Delta t}{\Delta x^2} & & & \\ D\frac{\Delta t}{\Delta x^2} & 1-2D\frac{\Delta t}{\Delta x^2} & & & \\ & \ddots & \ddots & \ddots & \\ & & D\frac{\Delta t}{\Delta x^2} & 1-2D\frac{\Delta t}{\Delta x^2} & D\frac{\Delta t}{\Delta x^2} \\ & & & D\frac{\Delta t}{\Delta x^2} & 1-2D\frac{\Delta t}{\Delta x^2} \end{pmatrix}. \tag{17.11}$$

We use the abbreviation

$$r = D\frac{\Delta t}{\Delta x^2} \tag{17.12}$$

and write A as

$$A = 1 + rM \tag{17.13}$$

with the tridiagonal matrix

$$M = \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}. \tag{17.14}$$

The eigenvalues of M are (compare (16.43))

$$\lambda = -4\sin^2\left(\frac{k}{2}\right) \text{ with } k = \frac{\pi}{N+1}, \frac{2\pi}{N+1}, \ldots \frac{N\pi}{N+1} \tag{17.15}$$

and hence the eigenvalues of A are given by

$$1 + r\lambda = 1 - 4r\sin^2\frac{k}{2}. \tag{17.16}$$

For stability we need

$$|1 + r\lambda| < 1 \quad \text{for all } \lambda \tag{17.17}$$

which holds if

$$-1 < 1 - 4r\sin^2\frac{k}{2} < 1. \tag{17.18}$$

The maximum of the sine function is $\sin\left(\frac{N\pi}{2(N+1)}\right) \approx 1$. Hence the right-hand inequation is fulfilled and from the left one we have

$$-1 < 1 - 4r \tag{17.19}$$

and finally stability for[1]

$$r = D\frac{\Delta t}{\Delta x^2} < \frac{1}{2}. \tag{17.20}$$

17.3.3 Implicit Backward Euler Algorithm

Consider now the implicit method

$$\begin{aligned} f(t_n, x_m) &= f(t_{n+1}, x_m) \\ &- D\frac{\Delta t}{\Delta x^2}(f(t_{n+1}, x_{m+1}) + f(t_{n+1}, x_{m-1}) - 2f(t_{n+1}, x_m)) - S(t_{n+1}, x_m)\Delta t \end{aligned} \tag{17.21}$$

or in matrix notation

$$f(t_n) = Af(t_{n+1}) - S(t_{n+1})\Delta t \quad \text{with } A = 1 - rM \tag{17.22}$$

which can be solved formally by

$$f(t_{n+1}) = A^{-1}f(t_n) + A^{-1}S(t_{n+1})\Delta t. \tag{17.23}$$

The eigenvalues of A are

$$\lambda = 1 + 4r\sin^2\frac{k}{2} > 1 \tag{17.24}$$

and the eigenvalues of A^{-1} are

$$\lambda^{-1} = \frac{1}{1 + r\sin^2\frac{k}{2}}. \tag{17.25}$$

The implicit method is stable since

$$|\lambda^{-1}| < 1. \tag{17.26}$$

[1] $m = \frac{\Delta t}{\Delta x^2}$ is the Courant number [89] for the diffusion equation.

17.3.4 Crank–Nicolson Method

Combination of implicit and explicit method gives the Crank–Nicolson method [93] which is often used for diffusion problems:

$$\begin{aligned}
&\frac{f(t_{n+1}, x_n) - f(t_n, x_n)}{\Delta t} \\
&= D\frac{f(t_n, x_{m+1}) + f(t_n, x_{m-1}) - 2f(t_n, x_m)}{2\Delta x^2} \\
&\quad + D\frac{f(t_{n+1}, x_{m+1}) + f(t_{n+1}, x_{m-1}) - 2f(t_{n+1}, x_m)}{2\Delta x^2} \\
&\quad + \frac{S(t_n, x_m) + S(t_{n+1}, x_m)}{2}\Delta t
\end{aligned} \tag{17.27}$$

or in matrix notation

$$\left(1 - \frac{r}{2}M\right) f(t_{n+1}) = \left(1 + \frac{r}{2}M\right) f(t) + \frac{S(t_n) + S(t_{n+1})}{2}\Delta t. \tag{17.28}$$

This can be solved for $f(t_{n+1})$:

$$f(t_{n+1}) = \left(1 - \frac{r}{2}M\right)^{-1} \left(1 + \frac{r}{2}M\right) f(t_n) + \left(1 - \frac{r}{2}M\right)^{-1} \frac{S(t_n) + S(t_{n+1})}{2}\Delta t. \tag{17.29}$$

The eigenvalues are now

$$\lambda = \frac{1 + \frac{r}{2}\mu}{1 - \frac{r}{2}\mu} \text{ with } \mu = -4\sin^2\frac{k}{2} = -4\cdots 0. \tag{17.30}$$

Since $r\mu < 0$ it follows

$$1 + \frac{r}{2}\mu < 1 - \frac{r}{2}\mu \tag{17.31}$$

and hence

$$\lambda < 1. \tag{17.32}$$

On the other hand we have

$$1 > -1 \tag{17.33}$$

$$1 + \frac{r}{2}\mu > -1 + \frac{r}{2}\mu \tag{17.34}$$

$$\lambda > -1. \tag{17.35}$$

which shows that the Crank–Nicolson method is stable [94].

17.3.5 Error Order Analysis

Taylor series expansion of $f(t+\Delta t, x) - f(t,x)$ gives for the explicit method

$$\begin{aligned}
&f(t+\Delta t, x) - f(t,x) = rMf(t,x) + S(t,x)\Delta t \\
&= D\frac{\Delta t}{\Delta x^2}\left(f(t,x+\Delta x) + f(t,x-\Delta x) - 2f(t,x)\right) + S(t,x)\Delta t. \qquad (17.36)
\end{aligned}$$

Making use of the diffusion equation we have

$$\begin{aligned}
&D\frac{\Delta t}{\Delta x^2}\left(\Delta x^2 f''(t,x) + \frac{\Delta x^4}{12}\frac{\partial^4}{\partial x^4}f(t,x) + \cdots\right) + S(t,x)\Delta t \\
&= \Delta t \dot{f}(t,x) + D\Delta t\frac{\Delta x^2}{12}\frac{\partial^4}{\partial x^4}f(t,x) + \cdots . \qquad (17.37)
\end{aligned}$$

For the implicit method we find

$$\begin{aligned}
&f(t+\Delta t, x) - f(t,x) = rMf(t+\Delta t,x) + S(t+\Delta t,x)\Delta t \\
&= D\frac{\Delta t}{\Delta x^2}\left(f(t+\Delta t,x+\Delta x) + f(t+\Delta t,x-\Delta x) - 2f(t+\Delta t,x)\right) \\
&\quad + S(t+\Delta t,x)\Delta t \\
&= D\frac{\Delta t}{\Delta x^2}\left(\Delta x^2 f''(t,x) + \frac{\Delta x^4}{12}f^{(4)}(t,x) + \cdots\right) \\
&\quad + S(t,x)\Delta t + D\frac{\Delta t^2}{\Delta x^2}\left(\Delta x^2 \dot{f}''(t,x) + \frac{\Delta x^4}{12}\dot{f}^{(4)}(t,x) + \cdots\right) + \dot{S}(t,x)\Delta t^2 \\
&= \Delta t\dot{f}(t,x) + \Delta t^2\ddot{f}(t,x) + D\Delta t\frac{\Delta x^2}{12}\left(f^{(4)}(t,x) + \Delta t\dot{f}^{(4)}(t,x)\right) + \cdots . \qquad (17.38)
\end{aligned}$$

We compare with the exact Taylor series

$$f_{\text{exact}}(t+\Delta t, x) - f(t,x) = \Delta t\dot{f}(t,x) + \frac{\Delta t^2}{2}\ddot{f}(t,x) + \frac{\Delta t^3}{6}\frac{\partial^3}{\partial t^3}f(t,x)\cdots \qquad (17.39)$$

and have for the explicit method

$$\begin{aligned}
&f_{\text{expl}}(t+\Delta t, x) - f(t,x) = \Delta t\dot{f}(t,x) + \frac{D\Delta x^2\Delta t}{12}f^{(4)}(t,x) + \cdots \\
&= f_{\text{exact}}(t+\Delta t,x) - f(t,x) + O(\Delta t^2, \Delta x^2\Delta t) \qquad (17.40)
\end{aligned}$$

and for the implicit method

$$\begin{aligned} f_{\text{impl}}(t+\Delta t, x) - f(t,x) &= \Delta t \dot{f}(t,x) + D\Delta t^2 \ddot{f}(t,x) + \cdots \\ &= f_{\text{exact}}(t+\Delta t, x) - f(t,x) + O(\Delta t^2, \Delta x^2 \Delta t). \end{aligned} \tag{17.41}$$

The error order of the Crank–Nicolson method is higher in Δt:

$$\begin{aligned} f_{\text{CN}}(t+\Delta t, x) - f(t,x) &= \frac{f_{\text{expl}}(t+\Delta t, x) - f(t,x)}{2} + \frac{f_{\text{impl}}(t+\Delta t, x) - f(t,x)}{2} \\ = \Delta t \dot{f}(t,x) + \frac{\Delta t^2}{2}\ddot{f}(t,x) + \cdots &= f_{\text{exact}}(t+\Delta t, x) - f(t,x) + O(\Delta t^3, \Delta x^2 \Delta t). \end{aligned} \tag{17.42}$$

17.3.6 Practical Considerations

For the implicit (17.22) and the Crank–Nicolson (17.29) method formally a tridiagonal matrix has to be inverted. However, it is numerically much more efficient to solve the tridiagonal systems of equations:

$$(1 - rM) f(t_{n+1}) = f(t_n) + S(t_{n+1})\Delta t \tag{17.43}$$

$$\left(1 - \frac{r}{2}M\right) f(t_{n+1}) = \left(1 + \frac{r}{2}M\right) f(t_n) + \frac{S(t_n) + S(t_{n+1})}{2}\Delta t$$

which can be done with the methods discussed in Part I on page 53.

17.3.7 Split Operator Method for $d > 1$ Dimensions

The simplest discretization of the Laplace operator in three dimensions is given by

$$\begin{aligned} \Delta f &= \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \\ &= \frac{1}{\Delta x^2}(\mathrm{d}_x^2 + \mathrm{d}_y^2 + \mathrm{d}_z^2) f, \end{aligned} \tag{17.44}$$

where

$$\frac{1}{\Delta x^2}\mathrm{d}_x^2 f = \frac{f(x+\Delta x, y, z) + f(x - \Delta x, y, z) - 2f(x,y,z)}{\Delta x^2}, \tag{17.45}$$

etc., denote the discretized second derivatives. Generalization of the Crank–Nicolson method for the three-dimensional problem gives

$$f(t_{n+1}) = \left(1 - \frac{r}{2}\mathrm{d}_x^2 - \frac{r}{2}\mathrm{d}_y^2 - \frac{r}{2}\mathrm{d}_z^2\right)^{-1} \left(1 + \frac{r}{2}\mathrm{d}_x^2 + \frac{r}{2}\mathrm{d}_y^2 + \frac{r}{2}\mathrm{d}_z^2\right) f(t). \tag{17.46}$$

But now the matrices $M_{x,y,z}$ representing the operators $d^2_{x,y,z}$ are not tridiagonal. To keep the advantages of tridiagonal matrices we use the approximations

$$\left(1+\frac{r}{2}\mathrm{d}_x^2+\frac{r}{2}\mathrm{d}_y^2+\frac{r}{2}\mathrm{d}_z^2\right)\approx\left(1+\frac{r}{2}\mathrm{d}_x^2\right)\left(1+\frac{r}{2}\mathrm{d}_y^2\right)\left(1+\frac{r}{2}\mathrm{d}_z^2\right) \tag{17.47}$$

$$\left(1-\frac{r}{2}\mathrm{d}_x^2-\frac{r}{2}\mathrm{d}_y^2-\frac{r}{2}\mathrm{d}_z^2\right)\approx\left(1-\frac{r}{2}\mathrm{d}_x^2\right)\left(1-\frac{r}{2}\mathrm{d}_y^2\right)\left(1-\frac{r}{2}\mathrm{d}_z^2\right) \tag{17.48}$$

and rearrange the factors to obtain

$$f(t_{n+1})=\left(1-\frac{r}{2}\mathrm{d}_x^2\right)^{-1}\left(1+\frac{r}{2}\mathrm{d}_x^2\right)\left(1-\frac{r}{2}\mathrm{d}_y^2\right)^{-1}\left(1+\frac{r}{2}\mathrm{d}_y^2\right)\left(1-\frac{r}{2}d_z^2\right)^{-1}\left(1+\frac{r}{2}\mathrm{d}_z^2\right)f(t_n) \tag{17.49}$$

which represents successive application of the one-dimensional method for the three directions separately. The last step was possible since operators d_i^2 and d_j^2 for different directions $i \neq j$ commute. For instance,

$$\begin{aligned}\mathrm{d}_x^2\mathrm{d}_y^2 f &= \mathrm{d}_x^2(f(x,y+\Delta x)+f(x,y-\Delta x)-2f(x,y))\\ &= f(x+\Delta x,y+\Delta y)+f(x-\Delta x,y+\Delta x)\\ &\quad -2f(x,y+\Delta x)+f(x+\Delta x,y-\Delta x)\\ &\quad +f(x-\Delta x,y-\Delta x)-2f(x,y-\Delta x)\\ &\quad -2f(x+\Delta x,y)-2f(x-\Delta x,y)+4f(x,y)\\ &= \mathrm{d}_y^2\mathrm{d}_x^2 f.\end{aligned} \tag{17.50}$$

The Taylor series of (17.46) and (17.49) coincides up to second order with respect to $r\mathrm{d}^2_{x,y,z}$:

$$\begin{aligned}&\left(1-\frac{r}{2}\mathrm{d}_x^2-\frac{r}{2}\mathrm{d}_y^2-\frac{r}{2}\mathrm{d}_z^2\right)^{-1}\left(1+\frac{r}{2}\mathrm{d}_x^2+\frac{r}{2}\mathrm{d}_y^2+\frac{r}{2}\mathrm{d}_z^2\right)\\ &=1+r(\mathrm{d}_x^2+\mathrm{d}_y^2+\mathrm{d}_z^2)+\frac{r^2}{2}(\mathrm{d}_x^2+\mathrm{d}_y^2+\mathrm{d}_z^2)^2+O(r^3)\end{aligned} \tag{17.51}$$

$$\begin{aligned}&\left(1-\frac{r}{2}\mathrm{d}_x^2\right)^{-1}\left(1+\frac{r}{2}\mathrm{d}_x^2\right)\left(1-\frac{r}{2}\mathrm{d}_y^2\right)^{-1}\left(1+\frac{r}{2}\mathrm{d}_y^2\right)\left(1-\frac{r}{2}\mathrm{d}_z^2\right)^{-1}\left(1+\frac{r}{2}\mathrm{d}_z^2\right)\\ &=\left(1+r\mathrm{d}_x^2+\frac{r^2\mathrm{d}_x^4}{2}\right)\left(1+r\mathrm{d}_y^2+\frac{r^2\mathrm{d}_y^4}{2}\right)\left(1+r\mathrm{d}_z^2+\frac{r^2\mathrm{d}_z^4}{2}\right)+O(r^3)\\ &=1+r(\mathrm{d}_x^2+\mathrm{d}_y^2+\mathrm{d}_z^2)+\frac{r^2}{2}(\mathrm{d}_x^2+\mathrm{d}_y^2+\mathrm{d}_z^2)^2+O(r^3).\end{aligned} \tag{17.52}$$

Hence we have

$$f_{n+1} = \left(1 + D\Delta t\left(\Delta + \frac{\Delta x^2}{12}\Delta^2 + \cdots\right) + \frac{D^2\Delta t^2}{2}(\Delta^2 + \cdots)\right) f_n$$
$$+ \left(1 + \frac{D\Delta t}{2}\Delta + \cdots\right)\frac{S_{n+1} + S_n}{2}\Delta t$$
$$= f_n + \Delta t(D\Delta f_n + S_n) + \frac{\Delta t^2}{2}(D^2\Delta^2 + D\Delta S_n + \dot{S}_n) + O(\Delta t\Delta x^2, \Delta t^3). \tag{17.53}$$

and the error order is conserved by the split operator method.

Problems

Problem 17.1 Diffusion in Two Dimensions

In this computer experiment we solve the diffusion equation on a two-dimensional grid for

- an initial distribution $f(t = 0, x, y) = \delta_{x,0}\delta_{y,0}$
- a constant source $f(t = 0) = 0,\ S(t, x, y) = \delta_{x,0}\delta_{y,0}$

Compare implicit, explicit, and Crank–Nicolson methods.