# Numerical methods for complex systems

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# Part I

# Partial Differential Equations

# Chapter 1

# Intorduction

## 1.1 Definition, Notation and Classification

A differential equation involving more than one independent variable and its (resp. their) partial derivatives with respect to those variables is called a *partial differential equation* (PDE).

Consider a simple PDE of the form:

$$\frac{\partial}{\partial x}u(x,y) = 0.$$

This equation implies that the function $u(x,y)$ is independent of $x$. Hence the general solution of this equation is $u(x,y) = f(y)$, where $f$ is an arbitrary function of $y$. The analogous ordinary differential equation is

$$\frac{du}{dx} = 0,$$

its general solution is $u(x) = c$, where $c$ is a constant. This example illustrates that general solutions of ODEs involve arbitrary constants, but solutions of PDEs, in contrast, involve *arbitrary functions*.

In general one can classify PDEs with respect to different criterion, e.g.:

- Order;
- Dimension;
- Linearity;
- Initial/Boundary value problem, etc.

By *order* of PDE we will understand the order of the highest derivative that occurs. A PDE is said to be *linear* if it is linear in unknown functions and their derivatives, with coefficients depending on the independent variables. The independent variables typically include one or more *space dimensions* and sometimes time dimension as well.
**Example:** The wave equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = a^2 \frac{\partial^2 u(x,t)}{\partial x^2}$$

is a one-dimensional, second-order linear PDE. In contrast, the Fisher Equation of the form

$$\frac{\partial u(\mathbf{r},t)}{\partial t} = \triangle u(\mathbf{r},t) + u(\mathbf{r},t) - u(\mathbf{r},t)^2,$$

where $\mathbf{r} = (x, y)$ is a two-dimensional, second-order nonlinear PDE.

## 1.2 Linear Second-Order PDEs

For linear equations in two dimensions there is a simple classification in terms of the general equation

$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu + g = 0,$$

where the coefficients $a, b, c, d, e, f$ and $g$ are real and in general can also be functions of $x$ and $y$. The PDE's of this type are classified by value of discriminant $D_\lambda = b^2 - 4ac$ of the eigenvalue problem for the matrix

$$A = \begin{pmatrix} a & b/2 \\ b/2 & c \end{pmatrix},$$

build from the coefficients of the highest derivatives. A simple classification is shown on the following table:

| $D_\lambda$ | Typ | Eigenvalues |
|---|---|---|
| $D_\lambda < 0$ | *elliptic* | the same sign |
| $D_\lambda > 0$ | *hyperbolic* | different signs |
| $D_\lambda = 0$ | *parabolic* | zero is an eigenvalue |

For instance, *the Laplace equation* for the electrostatic potential $\varphi$ in the space without a charge

$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0$$

is elliptic, as $a = c = 1$, $b = 0$, $D_\lambda = -4 < 0$. In general, elliptic PDEs describe processes that have already reached steady state, and hence are time-independent.

One-dimensional *wave equation* for some amplitude $A(x,t)$

$$\frac{\partial^2 A}{\partial t^2} - v^2 \frac{\partial^2 A}{\partial x^2} = 0$$

with the positive dispersion velocity $v$ is hyperbolic ($a = 1$, $b = 0$, $c = -v^2$, $D_\lambda = 4v^2 > 0$). Hyperbolic PDEs describe time-dependent, conservative processes, such as convection, that are not evolving toward steady state.

The next example is a diffusion equation for the patricle's density $\rho(x,t)$

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2},$$

where $D > 0$ is a diffusion coefficient is parabolic ($a = -D$, $b = c = 0$,$D_\lambda = 0$). Parabolic PDEs describe time-dependent, dissipative processes, such as diffusion, that are evolving toward steady state.

We shall consider each of these cases separately as different methods are required for each. The next point to emphasize is that as all the coefficients of the PDE can depend on $x$ and $y$ this classification concept is *local*.

## 1.3 Initial and Boundary-Value Problems

As it was mentioned above the solution of PDEs involve arbitrary functions. So, in order to solve the system in question completly, additional conditions are needed. These conditions can be given in the form of *initial* or *boundary* conditions. Initial conditions define the values of the dependent variables at the initial stage (e.g. at $t = 0$), whereas the boundary conditions give the information about the value of the dependent valiable or its derivative on the boundary of the area of interest. Typically, one distinguishes

- *Drichlet conditions* specify the values of the dependent variables of the boundary points.
- *Neumann conditions* specify the values of the normal gradients of the boundary.
- *Robin conditions* defines a linear combination of the Drichlet and Neumann conditions.

From the computational point of view it is useful to classify the PDE in question in terms of *initial value* or *boundary value problem*.

- *Initial value problem:* PDE in question describes *time evolution*, i.e., the initial space-distribution id given; the goal is to find how the dependent variable propagates in time. Example: The diffusion equation.

- *Boundary value problem:* A static solution of the problem should be found in some region-and the dependent variable is specified on its boundary. Example: The Laplace equation.

## 1.4 Finite difference method

Consider first a one-dimensional PDE for the unknown function $u(x,t)$. One way to numerically solve the PDE is to approximate all the derivatives by *finite differences*. We partition the domain in space using *a mesh* $x_0, x_1, \ldots, x_N$ and in time using a mesh $t_0, t_1, \ldots, t_T$. We assume first *a uniform partition* both in space and in time, so the difference between two consecutive space points will be $\triangle x$ and between two consecutive time points will be $\triangle t$, i.e.,

$$\begin{aligned} x_i &= x_0 + i\triangle x, \qquad i = 0, 1, \ldots, M; \\ t_j &= t_0 + j\triangle t, \qquad j = 0, 1, \ldots, T; \end{aligned}$$

### 1.4.1 The Taylor series method

Let us first consider a Taylor expansion of an analytical function $u$.

$$u(x+\triangle x) = u(x) + \sum_{n=1}^{\infty} \frac{\triangle x^n}{n!}\frac{\partial^n u}{\partial x^n} = u(x) + \triangle x\frac{\partial u}{\partial x} + \frac{\triangle x^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{\triangle x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots \tag{1.1}$$

Then for the first derivative one obtains:

$$\frac{\partial u}{\partial x} = \frac{u(x+\triangle x) - u(x)}{\triangle x} - \frac{\triangle x}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{\triangle x^2}{3!}\frac{\partial^3 u}{\partial x^3} - \ldots \tag{1.2}$$

If we break the right hand side of the last equation after the first term, for $\triangle x \ll 1$ the last equation becomes

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x+\triangle x) - u(x)}{\triangle x} + \mathcal{O}(\triangle x) = \frac{\triangle_i u}{\triangle x} + \mathcal{O}(\triangle x)}, \tag{1.3}$$

where

$$\triangle_i u = u(x+\triangle x) - u(x) = u_{i+1} - u_i$$

is called *a forward difference*. The backward expansion of the function $u$ can be written as $\triangle x \ll 1$ the last equation reads

$$u(x+(-\triangle x)) = u(x) - \triangle x\frac{\partial u}{\partial x} + \frac{\triangle x^2}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{\triangle x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots, \tag{1.4}$$

so for the first derivative one obtains

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x) - u(x-\triangle x)}{\triangle x} + \mathcal{O}(\triangle x) = \frac{\nabla_i u}{\triangle x} + \mathcal{O}(\triangle x)}, \tag{1.5}$$

where

$$\nabla_i u = u(x) - u(x-\triangle x) = u_i - u_{i-1}$$

is called *a backward difference*. if we substract Eq. (1.5) from Eq. (1.3) one obtains

$$u(x+\triangle x) - u(x-\triangle x) = 2\triangle x\frac{\partial u}{\partial x} + 2\frac{\triangle x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots, \tag{1.6}$$

what is equivalent to

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x+\triangle x) - u(x-\triangle x)}{2\triangle x} + \mathcal{O}(\triangle x^2)} \tag{1.7}$$

The second derivative can be found in the same way using the linear combination of different Taylor expansions. For instance, consider

$$u(x+2\triangle x) = u(x) + 2\triangle x\frac{\partial u}{\partial x} + \frac{(2\triangle x)^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{(2\triangle x)^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots \tag{1.8}$$

Substracting from the last equation Eq. (1.1), multiplied by two, one gets the following equation

$$u(x+2\triangle x) - 2u(x+\triangle x) = -u(x) + \frac{\triangle x^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{\triangle x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \ldots \tag{1.9}$$

So, one can approximate the second derivative as

$$\boxed{\frac{\partial^2 u}{\partial x^2} = \frac{u(x+2\triangle x) - 2u(x+\triangle x) + u(x)}{\triangle x^2} + \mathcal{O}(\triangle x).} \tag{1.10}$$

Similarly one can obtain the expression for the second derivative in terms of backward expansion, i.e.,

$$\boxed{\frac{\partial^2 u}{\partial x^2} = \frac{u(x-2\triangle x) - 2u(x-\triangle x) + u(x)}{\triangle x^2} + \mathcal{O}(\triangle x).} \tag{1.11}$$

Finally, if we add Eqn. (1.3) and 1.5 expression for the second derivative reads

$$\boxed{\frac{\partial^2 u}{\partial x^2} = \frac{u(x+\triangle x) - 2u(x) + u(x-\triangle x)}{\triangle x^2} + \mathcal{O}(\triangle x^2).} \tag{1.12}$$

In an analogous way one can obtain finite difference approximations to higher order derivatives and differential operators. The short overview of the forward, backward and central differences for first three derivatives can be found in Tables 1.1, 1.2, 1.3.

### 1.4.2 Mixed derivatives

A finite difference approximations for the mixed partial derivatives one get in the same way. For example, let us find the central approximation for the derivative

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right) = \frac{\partial}{\partial x}\left(\frac{u(x,y+\triangle y) - u(x,y-\triangle y)}{2\triangle y} + \mathcal{O}(\triangle y^2)\right) =$$
$$= \frac{u(x+\triangle x,y+\triangle y) - u(x-\triangle x,y+\triangle y) - u(x+\triangle x,y-\triangle y) + u(x-\triangle x,y-\triangle y)}{4\triangle x \triangle y} + \mathcal{O}(\triangle x^2 \triangle y^2)$$

### 1.4.3 A nonequidistant mesh

Let us suppose, that the spatial steps fulfill the following rule:

$$\triangle x_i = \alpha \triangle x_{i-1}.$$

If $\alpha = 1$ the mesh is said to be equidistant. Let us now calculate the first derivative of the function $u(x)$ of the second-order accurance.

$$u(x + \alpha\triangle x) = u(x) + \alpha\triangle x \frac{\partial u}{\partial x} + \frac{(\alpha\triangle x)^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{(\alpha\triangle x)^3}{3!}\frac{\partial^3 u}{\partial x^3} + \dots \tag{1.13}$$

Adding the last equation with Eq. (1.4) multiplied by $\alpha$ one obtains the expression for the second derivative

$$\frac{\partial^2 u}{\partial x^2} = \frac{u(x+\alpha\triangle x) - (1+\alpha)u(x) + \alpha u(x-\triangle x)}{\frac{1}{2}\alpha(\alpha+1)\triangle x^2} + \mathcal{O}(\triangle x) \tag{1.14}$$

After substitution of the last equation to Eq. (1.4) one obtains

$$\boxed{\frac{\partial u}{\partial x} = \frac{u(x+\alpha\triangle x) - (1-\alpha^2)u(x) - \alpha^2 u(x-\triangle x)}{\alpha(\alpha+1)\triangle x} + \mathcal{O}(\triangle x^2)} \tag{1.15}$$

| | $u_i$ | $u_{i+1}$ | $u_{i+2}$ | $u_{i+3}$ | $u_{i+4}$ |
|---|---|---|---|---|---|
| $\triangle x\frac{\partial u}{\partial x}$ | -1 | 1 | | | |
| $\triangle x^2\frac{\partial^2 u}{\partial x^2}$ | 1 | -2 | 1 | | |
| $\triangle x^3\frac{\partial^3 u}{\partial x^3}$ | -1 | 3 | -3 | 1 | |
| $\triangle x^4\frac{\partial^4 u}{\partial x^4}$ | 1 | -4 | 6 | -4 | 1 |

Table 1.1: Forward difference quotient, $\mathcal{O}(\triangle x)$

| | $u_{i-4}$ | $u_{i-3}$ | $u_{i-2}$ | $u_{i-1}$ | $u_i$ |
|---|---|---|---|---|---|
| $\triangle x\frac{\partial u}{\partial x}$ | | | | -1 | 1 |
| $\triangle x^2\frac{\partial^2 u}{\partial x^2}$ | | | 1 | -2 | 1 |
| $\triangle x^3\frac{\partial^3 u}{\partial x^3}$ | | -1 | 3 | -3 | 1 |
| $\triangle x^4\frac{\partial^4 u}{\partial x^4}$ | 1 | -4 | 6 | -4 | 1 |

Table 1.2: Backward difference quotient, $\mathcal{O}(\triangle x)$

| | $u_{i-2}$ | $u_{i-1}$ | $u_i$ | $u_{i+1}$ | $u_{i+2}$ |
|---|---|---|---|---|---|
| $2\triangle x\frac{\partial u}{\partial x}$ | | -1 | 0 | 1 | |
| $\triangle x^2\frac{\partial^2 u}{\partial x^2}$ | | 1 | -2 | 1 | |
| $2\triangle x^3\frac{\partial^3 u}{\partial x^3}$ | -1 | 2 | 0 | -2 | 1 |
| $\triangle x^4\frac{\partial^4 u}{\partial x^4}$ | 1 | -4 | 6 | -4 | 1 |

Table 1.3: Central difference quotient, $\mathcal{O}(\triangle x^2)$

## 1.5 Consistency, Convergence and Stability

### 1.5.1 Numerical Errors

*A numerical error* is either of two kinds of error in a calculation. The first (*a rounding error*) is caused by the finite precision of computations involving floating-point values. Increasing the number of digits allowed in a representation reduces the magnitude of possible roundoff errors, but any representation limited to finitely many digits will still cause some degree of roundoff error for uncountably many real numbers.

The second type of error (sometimes called *the truncation error*) is the difference between the exact mathematical solution and the approximate solution. Suppose, that we have defined an equidistant mesh $\{x_i\}$ and let us consider first a local error which arises from only one step of some numerical scheme.

A difference

$$\boxed{\varepsilon_{i+1} = u(x_{i+1}) - u_{i+1}} \tag{1.16}$$

is said to be *a local discretization error* in the point $x_{i+1}$. Here $u(x_{i+1})$ is a exact solution of the problem in the point $x_{i+1}$ whereas $u_{i+1}$ describes a value in this point, calculated using the numerical approximation. In other words, the local discretization error can be interpreted as a residuum, if one put the numerical solution into the exact one. Now, if we put the Taylor expansion in the vicinity of the point $(x_i, u(x_i))$ into the equation of interest, one get the information how fast the local error tends to zero with the spacing $\triangle x$. This observation leads to the definition of the so-called *consistency order*:

*One says, that a numerical scheme possess a consistency order p, if*

$$|\varepsilon_{i+1}| \leq C \triangle x^{p+1}, \quad i = 0, 1, 2, \ldots, \tag{1.17}$$

*where C is a constant.*

As mentioned above, the local error gives information about the accuracy of the numerial scheme, i.e., about the error in one its step. At the end of calculation one can calculate *an accumulated or a global discretization error* in tghe point $x_{i+1}$:

$$\boxed{e_{i+1} = u(x_{i+1}) - u_{i+1}.} \tag{1.18}$$

The value of the global error gives information about *convergence* of the approximation to the exact solution of the problem if the spacing value $\triangle x$ tends to zero, i.e.,

*A numerical scheme is said to be convergent, if for the global error* $e_i$ *one can write*

$$\max_{i=1\ldots n} |e_i| \to 0 \quad for \triangle x \to 0. \tag{1.19}$$

*The scheme posseses a convergence order p, if*

$$\max_{i=1\ldots n} |e_i| \leq C \triangle x^p, \tag{1.20}$$

*where C is a constant.*
**Notice:** At a first glance the global error tends to zero with the decreasing of $\triangle x$, so the mesh should be refined. However, decreasing of $\triangle x$ leads to the increasing of the rounding error. Another point to emphasize is that decreasing of $\triangle x$ can lead to *instability* of the numerical scheme in question. The notation of stability will be the topic of the next section.

### 1.5.2 Stability

An algorithm for solving an evolutionary partial differential equation is said to be *stable* if the numerical solution at a fixed time remains bounded as the step size goes to zero, so the pertrubations in form of, e.g., rounding error does not increase in time. Unfortunately, there are no general methods to verify the numerical stability for the partial differential equations in general form, so one restrict oneself to the case of linear PDE's. The standard method for linear PDE's was proposed by John von Neumann in 1947 and is based on the representation of the rounding error in form of the Foirer series.

#### von Neumann stability analysis

Consider the following notation:

$$u^{j+1} = \mathcal{T}[u^j]. \tag{1.21}$$

Here $\mathcal{T}$ is a nonlinear operator, depending on numerical scheme in question. The successive application of $\mathcal{T}$ results in a consequence of values

$$u^{(0)},\, u^{(1)},\, u^{(2)}, \ldots,$$

that approximate the exact solution of the problem. As was mentioned above, at each time step we add a small error $\varepsilon^{(j)}$, i.e.,

$$u^{(0)} + \varepsilon^{(0)},\, u^{(1)} + \varepsilon^{(1)},\, u^{(2)} + \varepsilon^{(2)}, \ldots,$$

where $\varepsilon^{(j)}$ is a cumulative rounding error at time $t_j$. Thus we obtain

$$u^{(j+1)} + \varepsilon^{(j+1)} = \mathcal{T}(u^{(j)} + \varepsilon^{(j)}) \tag{1.22}$$

After linearization of the last equation (we suppose that Taylor expansion for $\mathcal{T}$ is possible) the linear equation for the pertrubation takes the form:

$$\boxed{\varepsilon^{(j+1)} = \frac{\partial \mathcal{T}(u^{(j)})}{\partial u^{(j)}} \varepsilon^{(j)} := G\varepsilon^{(j)}} \tag{1.23}$$

This equation is called *error propagation law*, whereas the linearization matrix $G$ is said to be *an amplification matrix*. The stability of the numerical scheme depends now on the eigenvalues $g_\mu$ of $G$. In other words, the scheme is stable if and only if

$$|g_\mu| \leq 1 \quad \forall \mu$$

The question now is how this information can be used in practice. The first point to emphasize is that in general one deals with the $u(x_i, t_j) := u_i^(j)$, so one can write

$$\varepsilon_i^{(j+1)} = \sum_{i'} G_{ii'} \varepsilon_{i'}^{(j)}, \tag{1.24}$$

where

$$G_{ii'} = \frac{\partial \mathcal{T}(u^{(j)})_i}{\partial u_{i'}^{(j)}}.$$

For the values $\varepsilon_i^{(j)}$ (rounding error at the time step $t_j$ in the point $x_i$) one can display as a Fourier series:

$$\varepsilon_i^{(j)} = \sum_k e^{Ikx_j} \tilde{\varepsilon}^{(j)}(k), \tag{1.25}$$

where $I$ depicts the imagimary unit whereas $\tilde{\varepsilon}^{(j)}(k)$ are the Fourier coefficients. An important point is, that the functions $e^{Ikx_j}$ are eigenfunctions of the matrix $G$, so the last expansion can be interpreted as the expansion in eigenfunctions of $G$. Thus, for the practical point of view one take the error $\varepsilon_i^{(j)}$ just exact as

$$\varepsilon_i^{(j)} = e^{Ikx_j}.$$

The substitution of this expression into the Eq. (1.24) results in the following relation

$$\varepsilon_i^{(j+1)} = g(k) e^{Ikx_j} = g(k) \varepsilon_i^{(j)}. \tag{1.26}$$

Thus $e^{Ikx_j}$ is an eigenvector corresponding to the eigenvalue $g(k)$. The value $g(k)$ is often called *an amplification factor*. Finally, the stability criterium is given as

$$\boxed{|g(k)| \leq 1 \quad \forall k} \tag{1.27}$$

This criterium is called *von Neumann stablity criterium*.

# Chapter 2

# Hyperbolic PDE's

## 2.1 Wave equation

The wave equation is a second-order linear PDE that describes the propagation of a variety of waves, such as sound waves, light waves or water waves. It arises in different fields such as acoustics, electromagnetics, and fluid dynamics. The wave equation is the example of a hyperbolic PDE. In its simplest form, the wave equation refers to a scalar function $u = u(\mathbf{r}, t)$, $\mathbf{r} \in \mathbb{R}^n$ that satisfies:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u. \tag{2.1}$$

Here $\nabla^2$ denotes the Laplacian and $c$ is a constant speed of the wave propagation.

### 2.1.1 Wave equation in 1D

The wave equation for the scalar $u$ in the one dimensional case reads

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. \tag{2.2}$$

The general solution of Eq. (2.2) was first derived by *Jean le Rond d'Alembert*. Let us introduce new coordinates $(\xi, \eta)$ by use of the transformation

$$\xi = x - ct, \qquad \eta = x + ct. \tag{2.3}$$

In the new coordinate system Eq. (2.2) becomes

$$\frac{\partial^2 u}{\partial \xi \partial \eta} = 0. \tag{2.4}$$

This equation means that the function $u$ remains constant along the curves (2.3), i.e., (2.3) are characteristic curves of the wave equation (2.2). Moreover, one can see that the derivative $\partial u/\partial\xi$ does not depends on $\eta$, i.e.,

$$\frac{\partial}{\partial\eta}\left(\frac{\partial u}{\partial\xi}\right) = 0 \Leftrightarrow \frac{\partial u}{\partial\xi} = f(\xi). \tag{2.5}$$

After integration with respect to $\xi$ one obtains

$$u(\xi,\eta) = F(\xi) + G(\eta),$$

where $F$ is the primitive function of $f$ and $G$ is the "constant" of integration, in general the function of $\eta$. Turning back to the coordinates $(x,t)$ one obtains the general solution of Eq. (2.2)

$$\boxed{u(x,t) = F(x-ct) + G(x+ct).} \tag{2.6}$$

**Solution of the initial value problem**

Consider now an initial value problem for Eq. (2.2):

$$\begin{aligned} u_{tt} &= c^2 u_{xx}, \quad t \geq 0 \\ u(x,0) &= f(x), \\ u_t(x,0) &= g(x). \end{aligned} \tag{2.7}$$

To write down the general solution of the initial value problem for (2.2) one needs to exspress the arbitrary function $F$ and $G$ in terms of initial data $f$ and $g$. Using the relation

$$\frac{\partial}{\partial t}F(x-ct) = -cF'(x-ct), \quad \text{where} \quad F'(x-ct) := \frac{\partial}{\partial\xi}F(\xi)$$

one becomes:

$$\begin{aligned} u(x,0) &= F(x) + G(x) = f(x); \\ u_t(x,0) &= c(-F'(x) + G'(x)) = g(x). \end{aligned}$$

After differentiation of the first equation with respect to $x$ one can solve the system in terms of $F'(x)$ and $G'(x)$, i.e.,

$$F'(x) = \frac{1}{2}\big(f'(x) - \frac{1}{c}g(x)\big), \qquad G'(x) = \frac{1}{2}\big(f'(x) + \frac{1}{c}g(x)\big).$$

Hence

$$F(x) = \frac{1}{2}f(x) - \frac{1}{2c}\int_0^x g(y)dy + C, \quad G(x) = \frac{1}{2}f(x) + \frac{1}{2c}\int_0^x g(y)dy - C,$$

where the integration constant $C$ is chosen in such a way that the initial condition $F(x) + G(x) = f(x)$ is fullfield. Alltogether one obtains:

$$\boxed{u(x,t) = \frac{1}{2}\big(f(x-ct) + f(x+ct)\big) + \frac{1}{2c}\int_{x-ct}^{x+ct} g(y)dy} \tag{2.8}$$

### 2.1.2 A numerical scheme

Let us first consider initial value problem (2.7) for the one-dimensional wave equation (2.2).

#### An explicit method

The first idea is just to use central differences for both time and space derivatives, i.e.,

$$\frac{u_i^{j+1} - 2u_i^j + u_i^{j-1}}{\triangle t^2} = c^2 \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\triangle x^2} \tag{2.9}$$

or, with $\alpha = c\triangle t/\triangle x$

$$\boxed{u_i^{j+1} = -u_i^{j-1} + 2(1-\alpha^2)u_i^j + \alpha^2(u_{i+1}^j + u_{i-1}^j)} \tag{2.10}$$

Schematical representation of the scheme can be seen on Fig. 2.1.2.

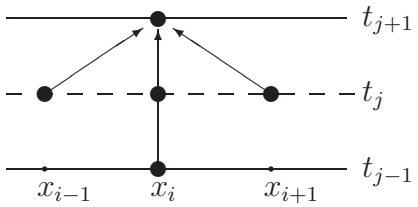


Figure 2.1: Schematical visualization of the numerical scheme (2.10) for (2.2).

Besides, one should add the initial conditions (2.7). To the implementation of the second initial condition one needs again the virtual point $u_i^{-1}$,

$$u_t(x_i, 0) = g(x_i) = \frac{u_i^1 - u_i^{-1}}{2\triangle t} + \mathcal{O}(\triangle t^2).$$

With $g_i := g(x_i)$ one can rewrite the last expression as

$$u_i^{-1} = u_i^1 - 2\triangle t g_i + \mathcal{O}(\triangle t^2),$$

and the second time row can be calculated as

$$\boxed{u_i^1 = \triangle t g_i + (1-\alpha^2)f_i + \frac{1}{2}\alpha^2(f_{i-1} + f_{i+1}),} \tag{2.11}$$

where $u(x_i, 0) = u_i^0 = f(x_i) = f_i$.

**Stability analysis**

The ansatz

$$\varepsilon_i^{j+1} = g^j e^{ikx_i}$$

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

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

which after some transformations becomes just a quadratic equation for $g$:

$$g^2 - 2\beta g + 1 = 0, \tag{2.12}$$

where

$$\beta = 1 - 2\alpha^2 \sin^2\big(\frac{k\triangle x}{2}\big).$$

Solutions read

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

If $\beta > 1$ then at least one of absolute value of $g_{1,2}$ is bigger that one. Therefor one should desire for $\beta < 1$, i.e.,

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

and

$$|g|^2 = \beta^2 + 1 - \beta^2 = 1.$$

In this case the scheme is *conditional stable*. The stability condition reads

$$-1 \leq 1 - 2\alpha^2 \sin^2\left(\frac{k\triangle x}{2}\right) \leq 1,$$

what is equivalent to the standart Courant-Friedrichs-Lewy-Condition

$$\alpha = \frac{c\triangle t}{\triangle x} \leq 1.$$

The number $\alpha$ is called *the Courant number*.

**An implicit method**

One can try to overcome the problems with conditional stability by introducing *an implicit scheme*. The simplest way to do it is just to replace all terms on the right hand side of (2.9) by an average from the values to the time steps $j+1$ and $j-1$, i.e,

$$\frac{u_i^{j+1} - 2u_i^j + u_i^{j-1}}{\triangle t^2} = \frac{c^2}{2\triangle x^2}\left(u_{i+1}^{j-1} - 2u_i^{j-1} + u_{i-1}^{j-1} + u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}\right). \tag{2.13}$$

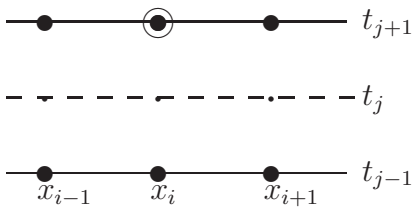


Figure 2.2: Schematical visualization of the implicit numerical scheme (2.13) for (2.2).

The schematical diagramm of the scheme (2.13) is shown on Fig. (2.1.2 )

Let us check the stability of (2.13). To this aim we use the standart ansatz

$$\varepsilon_i^{j+1} = g^j e^{ikx_i}$$

leading to the equation for $g(k)$

$$\beta g^2 - 2g + \beta = 0$$

with

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

One can see that $\beta \geq 1$ for all $k$. Hence the solutions $g_{1,2}$ take the form

$$g_{1,2} = \frac{1 \pm i\sqrt{1-\beta^2}}{\beta}$$

and

$$|g|^2 = \frac{1-(1-\beta^2)}{\beta^2} = 1.$$

Hence, the scheme (2.13) is *absolute stable*.

The question now is, whether the implicit scheme (2.13) is better than the explicit scheme (2.10) form numerical point of view. To answer this question, let us analyse dispersion relation for Eq. (2.2) as well as for both schemes (2.10) and (2.13). Exact dispersion relation is

$$\omega = \pm ck,$$

i.e, all Fourier modes propagate without dispersion with the same phase velocity $\omega/k = \pm c$.

Using the ansatz $u_i^j \sim e^{ikx_i - i\omega t_j}$ for the explicit method (2.10) one obtains:

$$\cos(\omega\triangle t) = 1 - \alpha^2(1 - \cos(k\triangle x)) \tag{2.14}$$

while for the implicit method (2.13)

$$\cos(\omega\triangle t) = \frac{1}{1+\alpha^2(1-\cos(k\triangle x))} \tag{2.15}$$

One can see that for $\alpha \to 0$ both methods provide the same result, otherwise

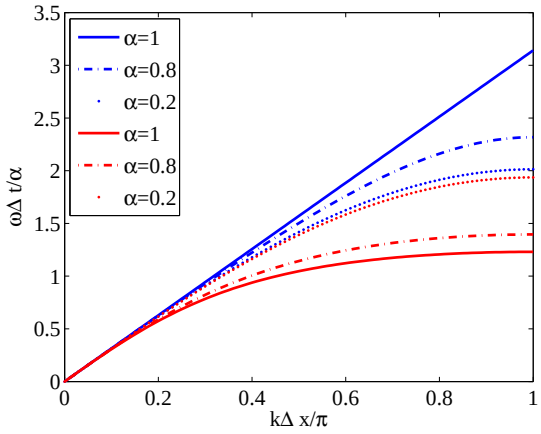


Figure 2.3: Dispersion relation for the explicit (blue curves) and implicit (red curves) methods.

the explicit scheme always exceeds the implicit one (see Fig. (2.1.2)). For $\alpha = 1$ the scheme (2.10) becomes exact, while (2.13) deviates more and more from the exact value of $\omega$ for increasing $\alpha$. Hence, there are no motivation to use implicit scheme instead of the explicit one.

### 2.1.3 Examples

**Example 1.**

Use the finite-difference method (2.10) to solve the wave equation for a vibrating string:

$$u_{tt} = 4u_{xx} \quad \text{for} \quad x \in [0,\, L] \quad \text{and} \quad t \in [0, T] \tag{2.16}$$

with the boundary conditions

$$u(0,t) = 0 \qquad u(L,t) = 0.$$

Assume that the initial position and velocity are

$$u(x,0) = f(x) = \sin(\pi x), \quad \text{and} \quad u_t(x,0) = g(x) = 0.$$

Other parameters are:

| | |
|---|---|
| `Space interval` | $L$=10 |
| `Space discretization step` | $\triangle x = 0.1$ |
| `Time discretization step` | $\triangle t = 0.05$ |
| `Amount of time steps` | $T = 20$ |

First one can find the d'Alambert solution. In the case of zero initial velocity Eq. (2.8) becomes

$$u(x,t) = \frac{f(x-2t) + f(x+2t)}{2} = \frac{\sin\pi(x-2t) + \sin\pi(x+2t)}{2} = \sin\pi x \cos 2\pi t,$$

i.e., the solution is just a sum of a travelling waves with initial form, given by $\frac{f(x)}{2}$. Numerical solution of (2.17) is shown on Fig. (2.1.3).

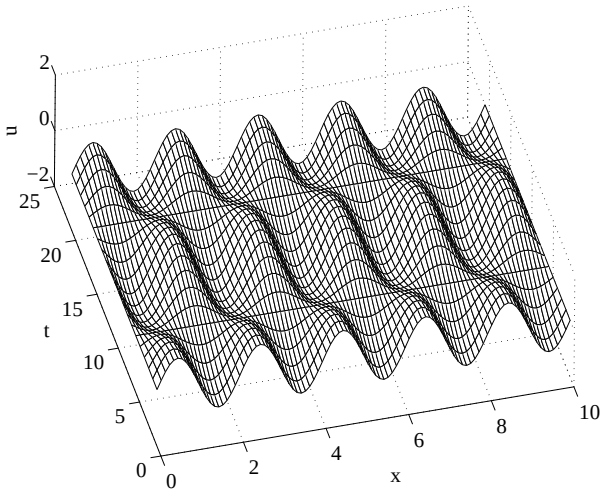


Figure 2.4: Space-time evolution of the initial distribution $u(x,0) = f(x)$, $u_t(x,0) = 0$.

**Example 2.**

Solve Eq. (2.17) with the same boundary conditions. Assume now, that initial distributions of position and velocity are

$$u(x,0) = f(x) = 0 \quad \text{and} \quad u_t(x,0) = g(x) = \begin{cases} 0, & x \in [0,\, x_1]; \\ g_0, & x \in [x_1,\, x_2]; \\ 0, & x \in [x_2,\, L]. \end{cases}$$

Other parameters are:

| | |
|---|---|
| `Initial nonzero velocity` | $g_0$=0.5 |
| `Initial space intervals` | $x_1 = L/4,\ x_2 = 3L/4$ |
| `Space interval` | $L$=10 |
| `Space discretization step` | $\triangle x = 0.1$ |
| `Time discretization step` | $\triangle t = 0.05$ |
| `Amount of time steps` | $T = 400$ |

Numerical solution of the problem is shown on Fig. (2.1.3).

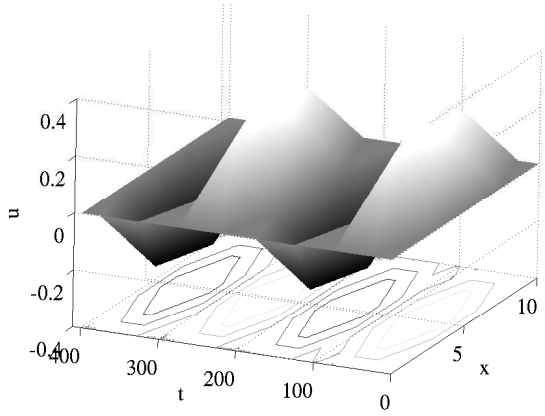


Figure 2.5: Space-time evolution of the initial distribution $u(x,0) = 0$, $u_t(x,0) = g(x)$.

**Example 3. Vibrating String**

Use the finite-difference method (2.10) to solve the wave equation for a vibrating string:

$$u_{tt} = c^2 u_{xx} \quad \text{for} \quad x \in [0,\, L] \quad \text{and} \quad t \in [0, T], \tag{2.17}$$

where $c = 1$ with the boundary conditions

$$u(0,t) = 0 \qquad u(L,t) = 0.$$

Assume that the initial position and velocity are

$$u(x,0) = f(x) = \sin(n\pi x/L), \quad \text{and} \quad u_t(x,0) = g(x) = 0, \quad n = 1, 2, 3, \ldots.$$

Other parameters are:

| | |
|---|---|
| `Space interval` | $L$=1 |
| `Space discretization step` | $\triangle x = 0.01$ |
| `Time discretization step` | $\triangle t = 0.0025$ |
| `Amount of time steps` | $T = 2000$ |

Usually a vibrating string produces a sound whose frequency is constant. Therefore, since frequency characterizes the pitch, the sound produced is a constant note. Vibrating strings are the basis of any string instrument like guitar or cello. If the speed of propagation $c$ is known, one can calculate the frequency of the sound produced by the string. The speed of propagation of a wave $c$ is equal to the wavelength multiplied by the frequency $f$:

$$c = \lambda f$$

If the length of the string is $L$, the fundamental harmonic is the one produced by the vibration whose nodes are the two ends of the string, so $L$ is half of the wavelength of the fundamental harmonic, so

$$f = \frac{c}{2L}$$

Solutions of the equation in question are given in form of standing waves. The standing wave is a wave that remains in a constant position. This phenomenon can occur because the medium is moving in the opposite direction to the wave, or it can arise in a stationary medium as a result of interference between two waves traveling in opposite directions (see Fig. (2.1.3))

### 2.1.4 Wave Equation in 2D

**Example 1.**

Use the standart five-point explicit method to solve a two-dimansional wave equation

$$u_{t,t} = c^2(u_{xx} + u_{yy}), \quad u = u(x, y, t)$$

on the rectangular domain $[0, L] \times [0, L]$ with Dirichlet boundary conditions. Other parameters are:

| | |
|---|---|
| `Space interval` | $L$=1 |
| `Space discretization step` | $\triangle x = \triangle y = 0.01$ |
| `Time discretization step` | $\triangle t = 0.0025$ |
| `Amount of time steps` | $T = 2000$ |
| `Initial condition` | $u(x, y, 0) = 4x^2y(1 - x)(1 - y)$ |

Solution for two different times can be seen on Fig. (**??**).

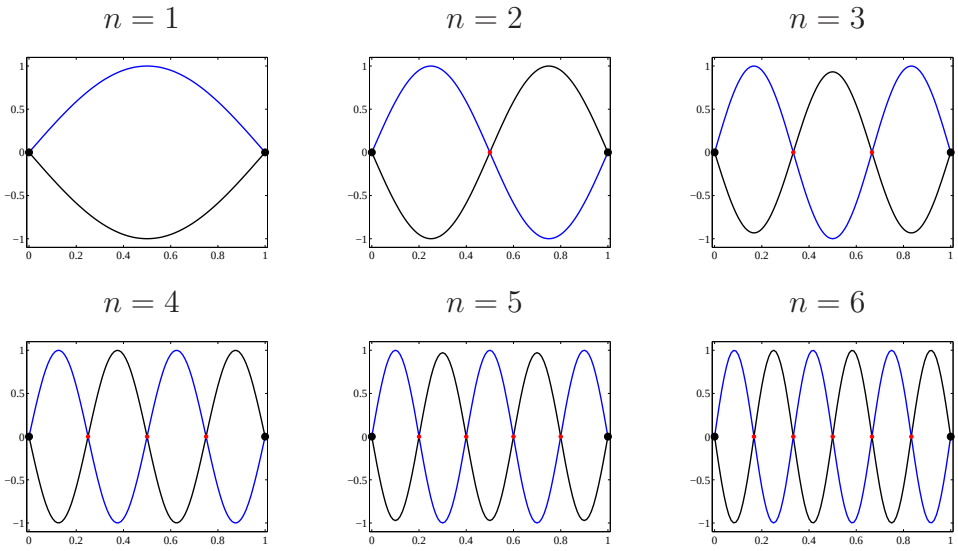


Figure 2.6: Standing waves in a string. The fundamental mode and the first five overtones are shown. The red dots represent the wave nodes.

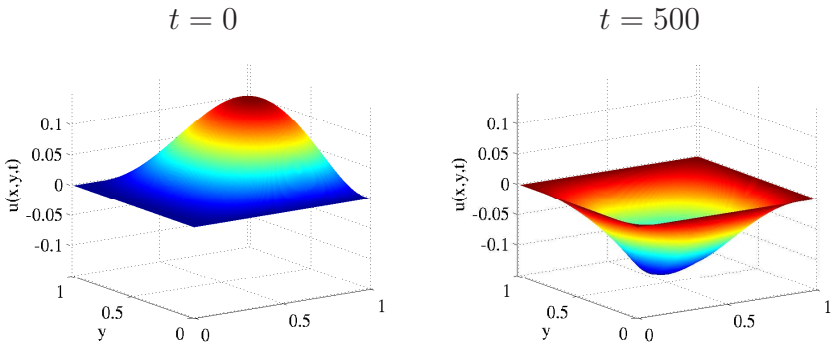


Figure 2.7: Numerical solution of the two-dimensional wave equation, shown on two different times.

## 2.2 Sine–Gordon equation

The sine-Gordon equation is a nonlinear hyperbolic partial differential equation involving the d'Alembert operator and the sine of the unknown function. It was originally considered in the nineteenth century in the course of study of surfaces of constant negative curvature. The equation grew greatly in importance when it was realized that it led to *solitons* ( so-called "kink" and "antikink"). The equation reads

$$u_{tt} - u_{xx} + \sin u = 0, \tag{2.18}$$

where $u = u(x,t)$. An interesting feature of the sine-Gordon equation is the existence of soliton and multisoliton solutions. If we look for localized waves of permanent profile of the form $u = u(\xi) = u(x - ct)$, such as $u \to 0$ and $du/d\xi \to 0$, when $\xi \to 0 \pm \infty$, the one-soliton solution can be calculated

$$u(x,t) = 4 \arctan\left(\exp\left(\pm\frac{x - ct}{\sqrt{1-c^2}}\right)\right). \tag{2.19}$$

Equation (2.19) represents a localized solitary wave, travelling at any velocity $|c| < 1$. The $\pm$ signs correspond to localized solutions which are called *kink* and *antikink* correspondenly (see Fig. 2.2).

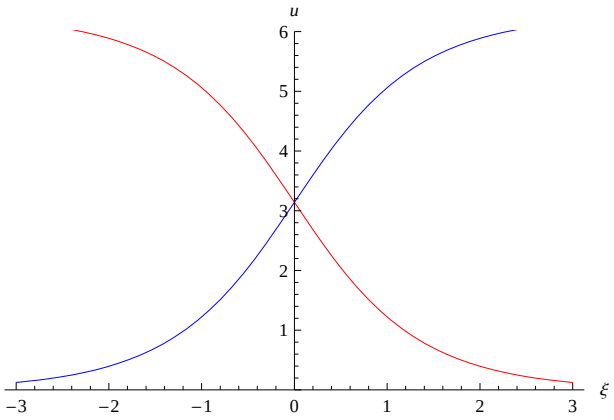


Figure 2.8: Representation of the kink (blue) and antikink (red) solutions (2.19)

The *kink-kink collision* solution has the form

$$u(x,t) = 4 \arctan\left(\frac{c \sinh\left(\frac{x}{\sqrt{1-c^2}}\right)}{\cosh\left(\frac{ct}{\sqrt{1-c^2}}\right)}\right) \tag{2.20}$$

and describes the collision between two kinks with respective velocities $c$ and $-c$ and approaching the origin from $t \to -\infty$ and moving away from it with velocities $\pm c$ for $t \to \infty$. Moreover, one can construct solution, corresponding

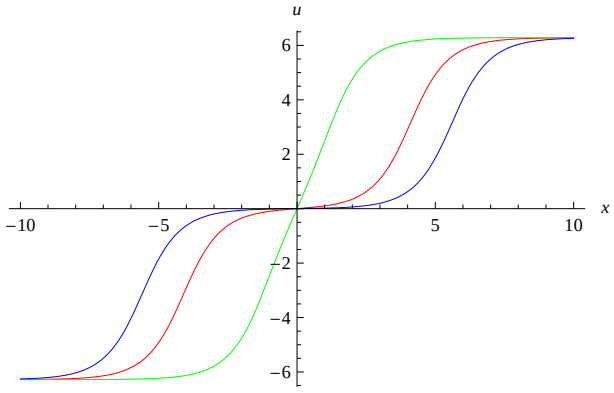


Figure 2.9: The kink-kink collision, calculated at three different times: At $t = -7$ (red curve) both kinks propagate with opposite velocities $c = \pm 0.5$; At $t = 0$ they collide at the origin (green curve); At $t = 10$ (blue curve) they move away from the origin with velocities $c = \mp 0.5$.

to the *kink-antikink coliision*. The solution reads:

$$u(x,t) = 4\arctan\left(\frac{\sinh\left(\frac{ct}{\sqrt{1-c^2}}\right)}{c\cdot\cosh\left(\frac{x}{\sqrt{1-c^2}}\right)}\right) \tag{2.21}$$

The *breather* soliton solution, which is also called a *breather mode* or *breather soliton*, is given by

$$u_B(x,t) = 4\arctan\left(\frac{\sqrt{1-\omega^2}\,\sin(\omega t)}{\omega\cosh(\sqrt{1-\omega^2}x)}\right) \tag{2.22}$$

which is periodic for frequencies $\omega < 1$ and decays exponentially when moving away from $x = 0$.

### 2.2.1 Numerical solution

#### A numerical scheme

Consider Eq. (2.18)

$$u_{tt} - u_{xx} + \sin(u) = 0$$

on the interval $x \in [a,\, b]$ with initial conditions

$$u(x,0) = f(x), \qquad u_t(x,0) = g(x) \tag{2.23}$$

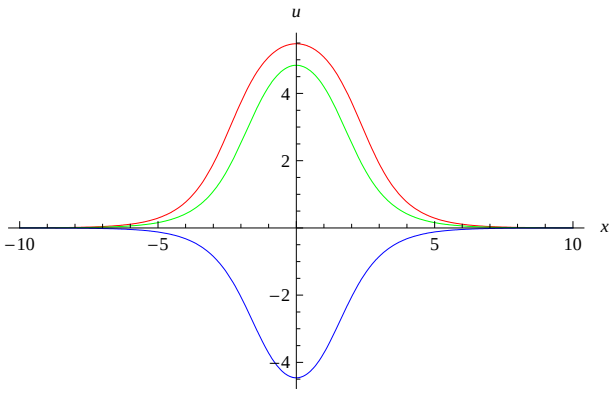


Figure 2.10: The breather solution, oscillating with the frequency $\omega = 0.2$ , calculated for three different times $t = 0$ (red curve), $t = 5$ (green curve) and $t = 10$ (blue curve).

and, e.g., no-flux boundary conditions

$$\left.\frac{\partial u}{\partial x}\right|_{x=a,b} = 0.$$

Let us try to apply a simple explicit scheme (2.10) to Eq. (2.18). The discretization scheme reads

$$u_i^{j+1} = -u_i^{j-1} + 2(1-\alpha^2)u_i^j + \alpha^2(u_{i+1}^j + u_{i-1}^j) - \triangle t^2 \sin(u_i^j) \tag{2.24}$$

with $\alpha = \triangle t/\triangle x$, $i = 0, \ldots, M$ and $t = 0, \ldots, T$.

To the implementation of the second initial condition one needs again the virtual point $u_i^{-1}$,

$$u_t(x_i, 0) = g(x_i) = \frac{u_i^1 - u_i^{-1}}{2\triangle t} + \mathcal{O}(\triangle t^2).$$

So, one can rewrite the last expression as

$$u_i^{-1} = u_i^1 - 2\triangle t g(x_i) + \mathcal{O}(\triangle t^2),$$

and the second time row can be calculated as

$$u_i^1 = \triangle t g(x_i) + (1-\alpha^2)f(x_i) + \frac{1}{2}\alpha^2(f(x_{i-1}) + f(x_{i+1})) - \frac{\triangle t^2}{2}\sin(f(x_i)). \tag{2.25}$$

No-flux boundary conditions lead to the expressions for two virtual space points $u^j_{-1}$ and $u^j_{M+1}$:

$$\begin{aligned}\left.\frac{\partial u}{\partial x}\right|_{x=a} &= 0 \Leftrightarrow \frac{u^j_1 - u^j_{-1}}{2\triangle x} = 0 \Leftrightarrow u^j_{-1} = u^j_1;\\ \left.\frac{\partial u}{\partial x}\right|_{x=b} &= 0 \Leftrightarrow \frac{u^j_M - u^j_{M+1}}{2\triangle x} = 0 \Leftrightarrow u^j_{M+1} = u^j_M;\end{aligned}$$

One can try to rewrite the differential scheme to more general matrix form. In matrix notation the second time-row is given by

$$\boxed{\mathbf{u}^1 = \triangle t\gamma_1 + A\mathbf{u}^0 - \frac{\triangle t^2}{2}\beta_1,} \tag{2.26}$$

where

$$\begin{aligned}\gamma_1 &= \big(g(a), g(x_1), g(x_2), \ldots, g(x_{M-1}), g(b)\big)^T \quad \text{and}\\ \beta_1 &= \big(\sin(u^0_0), \sin(u^0_1), \ldots, \sin(u^0_{M-1}), \sin(u^0_M)\big)^T\end{aligned}$$

are $M+1$-dimensional vectors and $A$ is a tridiagonal square $M+1 \times M+1$ matrix of the form

$$A = \begin{pmatrix} 1-\alpha^2 & \boxed{\alpha^2} & 0 & \ldots 0\\ \alpha^2/2 & 1-\alpha^2 & \alpha^2/2 & \ldots 0\\ 0 & \alpha^2/2 & 1-\alpha^2 & \ldots 0\\ \ldots & \ldots & \ldots & \ldots\\ 0 & \ldots & \boxed{\alpha^2} & 1-\alpha^2 \end{pmatrix}$$

The boxed elements indicate the influence of boundary conditions. Other time rows can also be written in the matrix form as

$$\boxed{\mathbf{u}^{j+1} = -\mathbf{u}^{j-1} + B\mathbf{u}^j - \triangle t^2\beta, \quad j = 1, \ldots, T-1} \tag{2.27}$$

Here

$$\beta = \big(\sin(u^j_0), \sin(u^j_1), \ldots, \sin(u^j_{M-1}), \sin(u^j_M)\big)^T$$

is a $M+1$-dimensional vector and $B$ is a square matrix, defined by an equation

$$B = 2A.$$

**Examples**

Solve Eq. (2.18) on the interval $[-L,\ L]$ using the following parameters:

| | |
|---|---|
| `Space interval` | $L$=20 |
| `Space discretization step` | $\triangle x = 0.1$ |
| `Time discretization step` | $\triangle t = 0.05$ |
| `Amount of time steps` | $T = 1800$ |
| `Velocity of the kink` | $c = 0.2$ |

Initial conditions are

a) *Kink solution:*

$$\begin{aligned} f(x) &= 4\arctan\Big(\exp\big(\frac{x}{\sqrt{1-c^2}}\big)\Big), \\ g(x) &= -2\frac{c}{\sqrt{1-c^2}}\mathrm{sech}\big(\frac{x}{\sqrt{1-c^2}}\big). \end{aligned}$$

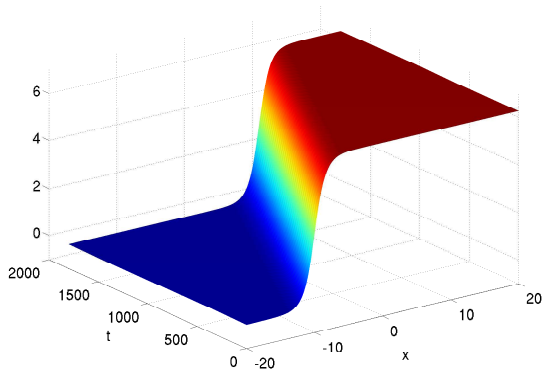


Figure 2.11: Space-time plot of the kink, moving with the velocity $c = 0.2$

b) *Antikink solution:*

$$\begin{aligned} f(x) &= 4\arctan\Big(\exp\big(-\frac{x}{\sqrt{1-c^2}}\big)\Big), \\ g(x) &= -2\frac{c}{\sqrt{1-c^2}}\mathrm{sech}\big(\frac{x}{\sqrt{1-c^2}}\big). \end{aligned}$$

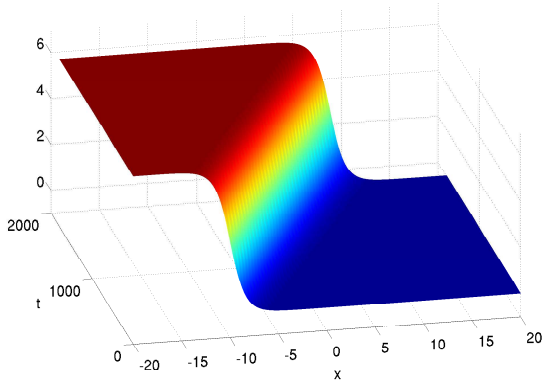


Figure 2.12: Space-time plot of the antikink, moving with the velocity $c = 0.2$

c) *Kink-kink colision:*

$$f(x) = 4\arctan\left(\exp\left(\frac{x+L/2}{\sqrt{1-c^2}}\right)\right) + 4\arctan\left(\exp\left(\frac{x-L/2}{\sqrt{1-c^2}}\right)\right),$$
$$g(x) = -2\frac{c}{\sqrt{1-c^2}}\text{sech}\left(\frac{x+L/2}{\sqrt{1-c^2}}\right) + 2\frac{c}{\sqrt{1-c^2}}\text{sech}\left(\frac{x-L/2}{\sqrt{1-c^2}}\right).$$

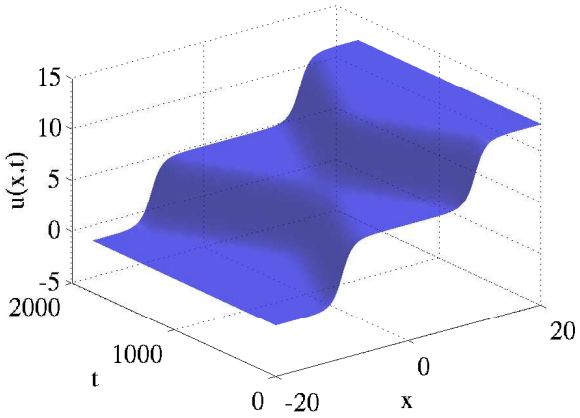


Figure 2.13: Space-time representation of kink-kink collision

d) *Kink-antikink colision:*

$$\begin{aligned} f(x) &= 4\arctan\Big(\exp\big(\frac{x+L/2}{\sqrt{1-c^2}}\big)\Big) + 4\arctan\Big(\exp\big(-\frac{x-L/2}{\sqrt{1-c^2}}\big)\Big), \\ g(x) &= -2\frac{c}{\sqrt{1-c^2}}\mathrm{sech}\big(\frac{x+L/2}{\sqrt{1-c^2}}\big) - 2\frac{c}{\sqrt{1-c^2}}\mathrm{sech}\big(\frac{x-L/2}{\sqrt{1-c^2}}\big). \end{aligned}$$

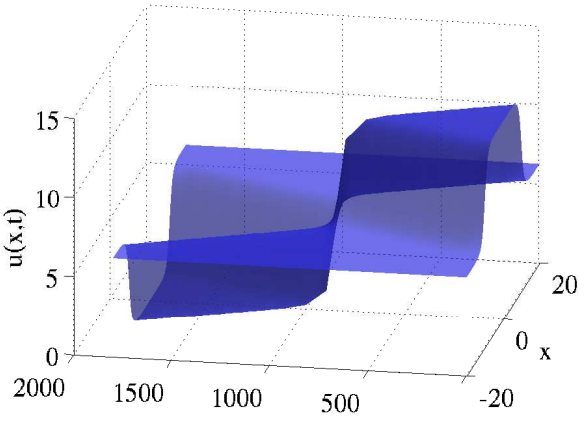


Figure 2.14: Space-time representation of kink-antikink collision

e) *Breather solution:*

$$\begin{aligned} f(x) &= 0, \\ g(x) &= 4\sqrt{1-c^2}\mathrm{sech}(x\sqrt{1-c^2}) \end{aligned}$$

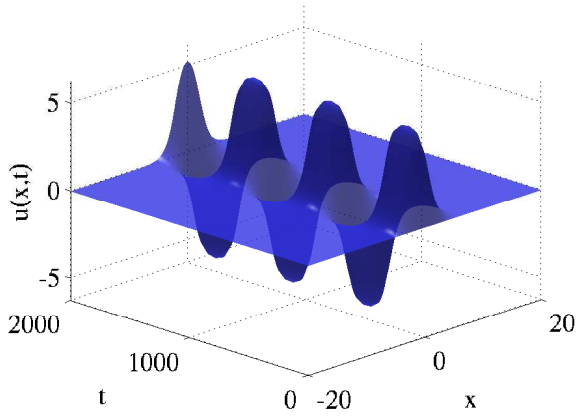


Figure 2.15: The breather solution, oscillating with the frequency $\omega = 0.2$

# Chapter 3

# Parabolic PDE's

## 3.1 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:

$$\frac{\partial u(\mathbf{r},t)}{\partial t} = \nabla \cdot \big(D(u(\mathbf{r},t),r)\nabla u(\mathbf{r},t)\big), \tag{3.1}$$

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. (3.1) reduces to the following linear equation:

$$\frac{\partial u(\mathbf{r},t)}{\partial t} = D\nabla^2 u(\mathbf{r},t). \tag{3.2}$$

Equation (3.2) is also called the *heat equation*, which describes the distribution of heat in a given region over time.

Equation (3.2) 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:

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

where $\mathbf{\Gamma}$ is the flux of the diffusing material. Equation (3.2) 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:

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

### 3.1.1 Diffusion equation in 1D

Consider the solution of the diffusion equation in one dimension:

$$\frac{\partial u(x,t)}{\partial t} = D\,\frac{\partial^2 u(x,t)}{\partial x^2} \tag{3.3}$$

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

$$u(x,0) = f(x), \qquad \forall\, x \in [0, L] \tag{3.4}$$

and Dirichlet boundary conditions

$$u(0,t) = u(L,t) = 0 \qquad \forall\, t > 0. \tag{3.5}$$

**Analytical solution**

Let us attempt to find a nontrivial solution of (3.3) satisfying the boundary conditions (3.5) using separation of variables, i.e., one makes an ansatz

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

Substituting $u$ back into Eq. (3.3) 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). Hence one can rewrite the last equation as a system of two ODE's:

$$X''(x) + \lambda X(x) = 0, \tag{3.6}$$
$$T'(t) + D\lambda T(t) = 0. \tag{3.7}$$

Taking into account boundary conditions (3.5) one obtains ($T(t) \neq 0$ as we are loocking for nontrivial solutions)

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

Hence the problem of finding of the solution reduces to the solving of linear ODE and consideration of three different cases with respect to the sign of $\lambda$:

1. $\lambda < 0$:
$$X(x) = C_1 e^{\sqrt{-\lambda}x} + C_2 e^{-\sqrt{-\lambda}x}.$$
Taking into account the boundary conditions one get $C_1 = C_2 = 0$, so only trivial solution exists for $\lambda < 0$.

2. $\lambda = 0$:
$$X(x) = C_1 x + C_2$$
With account of boundary conditions one gets again 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
$$X(t) = C_n \sin\big(\frac{\pi n}{L}x\big)$$

Then the equation for the function $T(t)$ takes the form:
$$T'(t) + D\big(\frac{\pi n}{L}\big)T(t) = 0 \Rightarrow T(t) = B_n \exp\big(-D\big(\frac{\pi n}{L}\big)^2 t\big),$$
where $B_n$ is constant. Altogether, the general solution of the problem can be written as
$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin\big(\frac{\pi n}{L}x\big) e^{-D\left(\frac{\pi n}{L}\right)^2 t}, \quad A_n = \text{const}.$$
In order to find $A_n$ one can use initial condition (3.4). 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. (3.3) reads:
$$\boxed{u(x,t) = \sum_{n=1}^{\infty}\left(\frac{2}{L}\int_0^L f(\xi)\sin\big(\frac{\pi n}{L}\xi\big)\, d\xi\right)\sin\big(\frac{\pi n}{L}x\big)e^{-D\left(\frac{\pi n}{L}\right)^2 t}.} \qquad (3.8)$$

### 3.1.2 Numerical methods

**A simple explicit method (FTCS)**

Consider Eq. (3.3) with initial condition (3.4). The first simple idea is a simple explicit FTCS method (*Forward in Time, Central in Space*) (see Fig. (3.1.2)):

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

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

$$\boxed{u_i^{j+1} = (1-2\alpha)u_i^j + \alpha(u_{i+1}^j + u_{i-1}^j)} \tag{3.9}$$

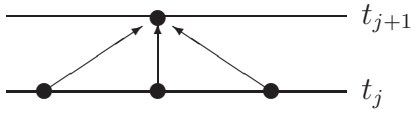


Figure 3.1: Schematical representation of the FTCS finite difference scheme for solving the 1-d diffusion equation

Applying the von Neumann analysis to this system by considering a single Fourier mode in $x$ space, we obtain the 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 condition that the method is stable for all $k$ gives

$$|g(k)| \leq 1 \quad \forall\, k \;\Leftrightarrow\; \alpha \leq \frac{1}{2} \;\Leftrightarrow\; \boxed{\triangle t \leq \frac{1}{2}\frac{\triangle x^2}{D}}. \tag{3.10}$$

Although the method (3.9) is in fact conditionally stable the stability condition (3.10) 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.

Another point to emphasize is the numerical dispersion. Indeed, let us compare the exact dispersion relation for Eq. (3.3) and relation, obtained by

means of (3.9). If we consider the perturbations in form $\exp(ikx - i\omega t)$ the dispersion relation for Eq. (3.3) reads

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

On the other hand, the FTCS scheme (3.3) 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 relations is shown on Fig. (3.1.2).

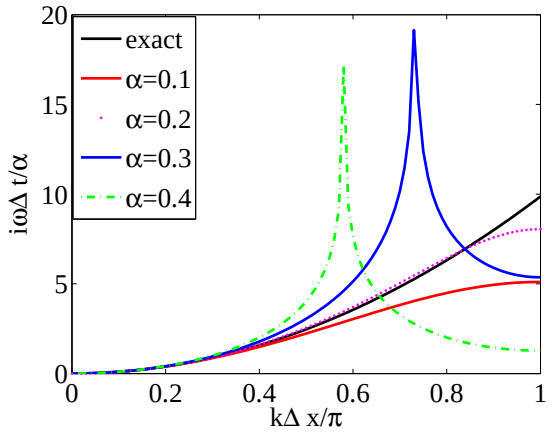


Figure 3.2: Dispersion relation by means of the scheme (3.9) for different values of $\alpha$, compared with the exact relation for Eq. (3.3).

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 $\omega$ can be complex, i.e., the Fourier modes drops off, performing damped oscillations (see Fig. (3.1.2) for $\alpha = 0.3$ and $\alpha = 0.4$). If we try now 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 as well.

### Richardson Method

The first ideais to try to improve the approximation order of the scheme using the central diferences for the time derivative as well, namely

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

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

$$\boxed{u_i^{j+1} = u_i^{j-1} + 2\alpha\big(u_{i+1}^j - 2u_i^j + u_{i-1}^j\big)} \tag{3.11}$$

Unfortunately, one can show that the scheme (3.11) is unconditional unstable. Indeed, amplification factor $g(k)$ in this case fulfills 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 $|g_2(k)| > 1 \quad \forall k$, the scheme (3.11) is unconditional unstable.

### 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. (3.9) to read (see Fig. (3.1.2))

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

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

$$\boxed{u_i^{j+1} = \frac{1-\alpha}{1+\alpha}u_i^{j-1} + \frac{\alpha}{1+\alpha}\big(u_{i+1}^j + u_{i-1}^j\big),} \tag{3.12}$$

where $\alpha = 2D\triangle t/\triangle x$.

When the usual von Neumann analysis is applied to (3.12), 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 $\alpha$, so the method (3.12) is unconditionally stable. However, this does not

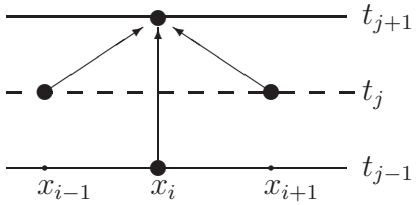


Figure 3.3: Schematical representation of the DuFort-Frankel method (3.12).

imply that $\triangle x$ and $\triangle t$ can be made indefinitely large; we must still worry about the accuracy of the method. Indeed, consider the Taylor expansion for Eq. (3.3) by means of (3.12):

$$\begin{aligned}
\frac{u_i^{j+1}-u_i^{j-1}}{2\triangle t} &= D\frac{u_{i+1}^j-u_i^{j+1}-u_i^{j-1}+u_{i-1}^j}{\triangle x^2} \Leftrightarrow \\
u_t-\frac{\triangle x^2}{3!}u_{ttt}+\ldots &= \frac{D}{\triangle x^2}\left(\triangle x^2 u_{xx}+\frac{2\triangle x^4}{4!}u_{xxxx}-\triangle t^2 u_{tt}-\frac{2\triangle t^4}{4!}u_{tttt}+\ldots\right) \Leftrightarrow \\
u_t+\mathcal{O}(\triangle t^2) &= Du_{xx}+\mathcal{O}(\triangle x^2)-D\left(\frac{\triangle t^2}{\triangle x^2}\right)u_{tt}+\mathcal{O}\left(\frac{\triangle t^4}{\triangle x^2}\right).
\end{aligned}$$

In other words, the method (3.12) has order of accuracy

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

For cosistency, $\triangle t/\triangle x \to 0$ as $\triangle t \to 0$ and $\triangle x \to 0$, so (3.12) is inconsistent. This constitutes an effective restriction on $\triangle t$. For large $\triangle t$, however, the scheme (3.12) is consistent with *another* equation of the form

$$Du_{tt}+u_t = Du_{xx}.$$

**A simple implicit method (BTCS)**

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 (3.1.2)). The differential scheme reads:

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

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

$$\boxed{-u_i^j = \alpha u_{i+1}^{j+1}-(1+2\alpha)u_i^{j+1}+\alpha u_{i-1}^{j+1}.} \tag{3.13}$$

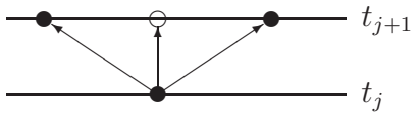


Figure 3.4: Schematical representation of the BTCS method (3.13).

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 scheme (3.13) is unconditionally stable. However, the method has order of accuracy $\mathcal{O}(\triangle t, \triangle x^2)$, i.e., first order in time, and second in space. Is it possible to improve it? The answer to is given below.

**Crank-Nicolson Method**

An implicit scheme, introduced by John Crank and Phyllis Nicolson in the mid 20th century is based on the central approximation of Eq. (3.3) at the point $(x_i,\, t_j + \frac{1}{2}\triangle t)$ (see Fig. (3.1.2)):

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

The approximation used for the space derivative is just an average of ap-

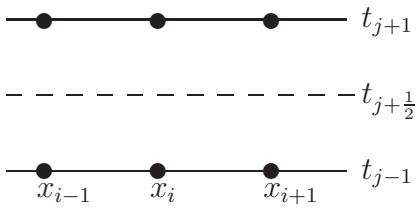


Figure 3.5: Schematical representation of the Crank-Nicolson method (3.14).

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

$$\boxed{-\alpha u_{i+1}^{n+1} + 2(1+\alpha)u_i^{n+1} - \alpha u_{i-1}^{n+1} = \alpha u_{i+1}^n + 2(1-\alpha)u_i^n + \alpha u_{i-1}^n.} \quad (3.14)$$

The terms on the right-hand side of Eq. (3.14) are all known. Hence the equations in (3.14) form a tridiagonal linear system $A\mathbf{u} = \mathbf{b}$. The amplification factor for Eq. (3.14) reads

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

Since $\alpha$ 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 (3.14) is unconditionaly stable.

### 3.1.3 Examples

Example 1: Use the FTCS explicit method to solve the one-dimensional heat equation

$$u_t = u_{xx},$$

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

| | |
|---|---|
| `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` | $f(x) = 4x(1 - x)$ |

Example 2: Use the Crank-Nicolson method 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 the temperature on both ends of the interval is given as $u(0, t) = T_l$, $u(L, t) = T_r$.

| | |
|---|---|
| `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` | $f(x) = 2 - 1.5x + \sin(\pi x)$ |

Solution of the problem is shown on Fig. (3.1.3).

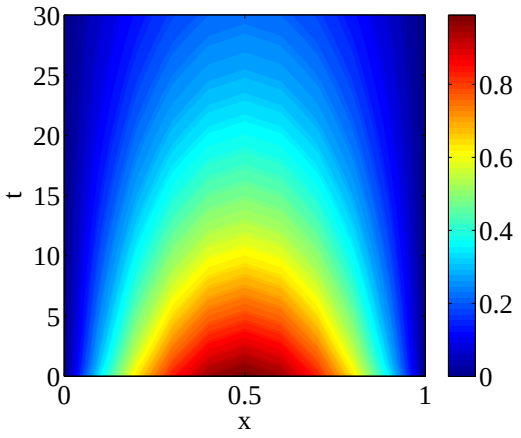


Figure 3.6: Contour plot of the heat distribution after the time $T = 30$, calculated with FTCS method.

Example 3: Use the implicit BTCS method 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 $u_x(-L,t) = u_x(L,t) = 0$.

| | |
|---|---|
| `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. (3.1.3).

## 3.2 Reaction-diffusion equations in 1D

Reaction-diffusion (RD) equations arise naturally in systems consisting of many interacting components, (e.g., chemical reactions) and are widely used to describe pattern-formation phenomena in variety of biological, chemical and physical systems. The principal ingredients of all these models are equation of the form

$$\partial_t \mathbf{u} = \mathbf{D}\nabla^2\mathbf{u} + \mathbf{R}(\mathbf{u}), \tag{3.15}$$

where $\mathbf{u} = \mathbf{u}(\mathbf{r},\mathbf{t})$ is a vector of concentration variables, $\mathbf{R}(\mathbf{u})$ describes as before a local reaction kinetics and the Laplace operator $\nabla^2$ acts on the

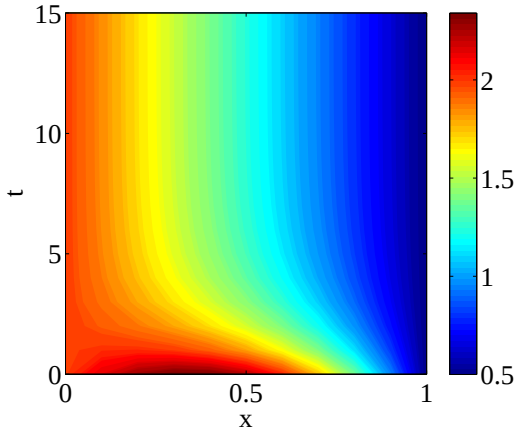


Figure 3.7: Contour plot of the heat distribution, calculated with the Crank-Nicolson method.

vector **u** componentwise. **D** denotes a diagonal diffusion coefficient matrix. Note that we suppose the system (3.15) to be isotropic and uniform, so **D** is represented by a scalar matrix, independent on coordinates.

In the following subsections we discuss different nontrivial solutions of this system for different number of components, starting with the case of one component RD system in one spatial dimension, namely

$$u_t = Du_{xx} + R(u),$$

where $D = \text{const}$. Suppose, that initial distribution $u(x, 0)$ is given on the whole space interval $x \in (-\infty, +\infty)$ and assume that

$$u(-\infty, t) = u_-, \qquad u(+\infty, t) = u_+,$$

where $u_\pm$ are stable steady state solutions of the equation in question,i.e, solutions of $R(u) = 0$.

### 3.2.1 FKPP-Equation

Investigation in this field starts form the classical papers of Fisher (1937) and Kolmogorov, Petrovsky and Piskunoff (1937) motivated by population dynamics issues, where authors arrived at a modified diffusion equation:

$$\partial_t u(x, t) = D\partial_x^2 u(x, t) + R(u), \tag{3.16}$$

with a nonlinear source term $R(u) = u - u^2$. A typical solution of the Eq. (3.16) is a propagating front, separating two non-equilibrium homogeneous states, one of which $(u = 1)$is stable and one of which $(u = 0)$ is

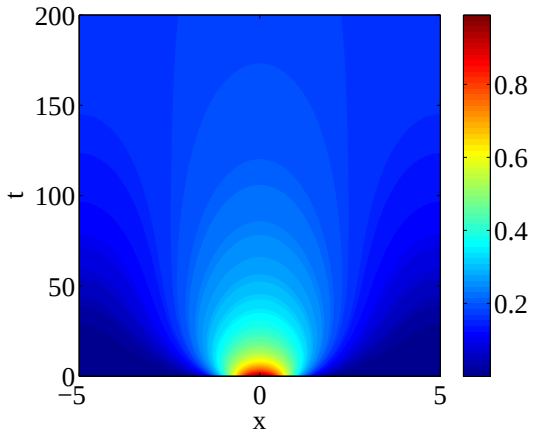


Figure 3.8: Contour plot of the diffusion of the initial Gauss pulse, calculated with the BTCS implicit method.

unstable. Such fronts behavior is often said to be *front propagation into unstable state* and fronts as such are referred to as *waves (or fronts) of transition from an unstable state*.

It is known that for Eq. (3.16) the propagating front always relaxes to a unique shape and velocity

$$c^* = 2\sqrt{D}, \tag{3.17}$$

if the initial profile is well-localized.

### Numerical method

Let us consider Eq. (3.16) and suppose that initial distribution $u(x,0) = f(x)$ as well as no-flux boundary conditions are given. We can try to apply an implicit BTCS-method for the linear part of the equation, taking the nonlinearilty explicitly, i.e.,

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

where $R(u_i^j) = u_i^j - (u_i^j)^2$. We can rewrite the last equation to the matrix form

$$A\mathbf{u^{n+1}} = \mathbf{u^n} + \triangle t \cdot R(\mathbf{u^n}), \tag{3.18}$$

where matrix $A$ is a tridiagonal $M+1 \times M+1$ matrix of the form

$$A = \begin{pmatrix} 1+2\alpha & \boxed{-2\alpha} & 0 & \dots 0 \\ -\alpha & 1+2\alpha & -\alpha & \dots 0 \\ 0 & -\alpha & 1+2\alpha & \dots 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & \boxed{-2\alpha} & 1+2\alpha \end{pmatrix},$$

$\alpha = D\triangle t/\triangle x^2$. The boxed elements indicate the influence of boundary conditions.

**Example**

Let us solve Eq. (3.16) on the interval $x \in [-L, L]$ with the method 3.18. Parameters are:

| | |
|---|---|
| `Space interval` | $L = 50$ |
| `Space discretization step` | $\triangle x = 0.2$ |
| `Time discretization step` | $\triangle t = 0.05$ |
| `Amount of time steps` | $T = 800$ |
| `Diffusion coefficient` | $D = 1$ |
| `Initial distribution` | $f(x) = 0.05e^{-5x^2}$ |

Numerical solution for six different times is shown on Fig. (3.2.1). One can

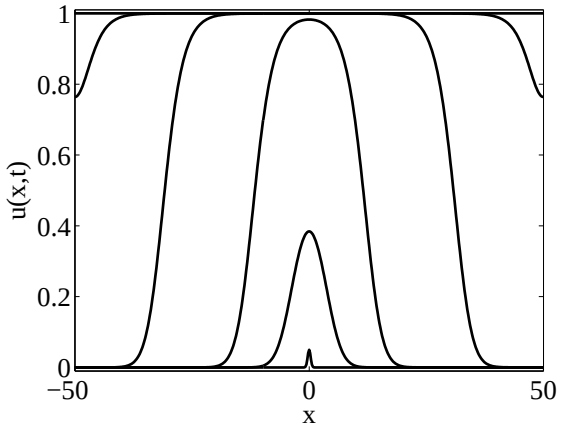


Figure 3.9: Numerical solution of (3.16) calculated with the method (3.18) for six different times $t = 0$, 100, 200, 400, 600, 800.

see, that a small local initial fluctuation leads to an instability, that develops in a nonlinear way: a front propagates away from the initial perturbation. Finally the uniform stable state with $u = 1$ is established on the whole space interval.

### 3.2.2 Switching waves

Another important class of one-component RD systems is so-called *bistable systems*. They possess two stable states, say $u = u_-$ and $u = u_+$, separated by an unstable state $u = u_0$. The fundamental form of a pattern in bistable infinite one-component media is *a trigger wave*, which represents a propagating front of transition from one stationary state into the other. In the literature other nomenclature, e.g., *switching waves* is also used. The propagation velocity of a flat front is uniquely determined by the properties of the bistable medium. Indeed, moving to a frame moving with a constant velocity $\xi := x - ct$, and considering partial solution of the form $u = u(\xi)$ one obtains equation

$$Du_{\xi\xi} + cu_\xi + R(u) = 0$$

with boundary conditions

$$u(\xi \to -\infty) = u_-, \qquad u(\xi \to +\infty) = u_+.$$

Introducing the potential $R(u) = \frac{\partial V(u)}{\partial u}$ one can show that in this situation the velocity of the front can be determined as

$$c = \frac{V(u_+) - V(u_-)}{\int\limits_{-\infty}^{+\infty} (u_\xi)^2 d\xi}.$$

The numerator of the last equation uniquely defines the velocity direction. In particular, if $V(u_+) = V(u_-)$ the front velocity equals zero, so *stationary front* is also a solution in bistable one-component media. However, the localized states in form of a domain, which can be produced by a connection of two fronts propagating in opposite directions, are normally unstable. Indeed, for the arbitrary choice of parameters one state ($V(u_+)$ or $V(u_-)$) will be dominated. This causes either collapse or expansion of the two-front solution.

#### Example 1: Zeldovich Equation

An example of bistable system is the Zeldovich–Frank–Kamenetsky–equation, describing, e.g., the flame propagation

$$u_t = Du_{xx} + u(1-u)(u-\beta), \quad \beta \in (0,\, 1). \tag{3.19}$$

Let us solve Eq. (3.20) on the interval $x \in [-L,\, L]$ with no-flux boundary conditions by means of numerical scheme (3.18). Other parameters are:

| | |
|---|---|
| `Space interval` | $L = 10$ |
| `Space discretization step` | $\triangle x = 0.04$ |
| `Time discretization step` | $\triangle t = 0.05$ |
| `Amount of time steps` | $T = 150$ |
| `Diffusion coefficient` | $D = 1$ |

Consider four different cases:

a) Moving fronts: $\beta = 0.8$;

b) Moving fronts: $\beta = 0.1$ Initial distribution:

$$u(x,0) = \begin{cases} u_-, & \text{for} \quad x \in [-L, 0] \\ u_+, & \text{for} \quad x \in (0, L] \end{cases}$$

c) Front collision: $\beta = 0.8$;

d) Front scattering: $\beta = 0.1$ Initial distribution:

$$u(x,0) = \begin{cases} u_-, & \text{for} \quad x \in [-L, -L/3] \\ u_+, & \text{for} \quad x \in (-L/3, L/3) \\ u_-, & \text{for} \quad x \in [L/3, L] \end{cases}$$

Results of the numerical calculation is shown on Fig. (3.2.2).

**Example 2: Stationary fronts**

Consider a one-dimensional RD equation, describing a bistable media

$$u_t = Du_{xx} + u(1 - u^2), \tag{3.20}$$

$x \in [-L, L]$. Equation (3.20) has three steady state solutions: two stable $u_\pm = \pm 1$, separated with an unstable state $u_0 = 0$. One can calculate the potential values at $u = u_\pm$,

$$V(u_-) = V(u_+) \Rightarrow c = 0.$$

That is, a stationary front, connecting stable steady state is expected to be a solution. Moreover, one can constuct a localized pulse by a connection of two stable fronts. The form of the stationary front can be found analytically, namely

$$u(x) = \tanh\left(\frac{x - x_0}{\sqrt{2D}}\right).$$

From numerical point of view one can use the scheme (3.18) for $R(u) = u - u^3$. Parameters are

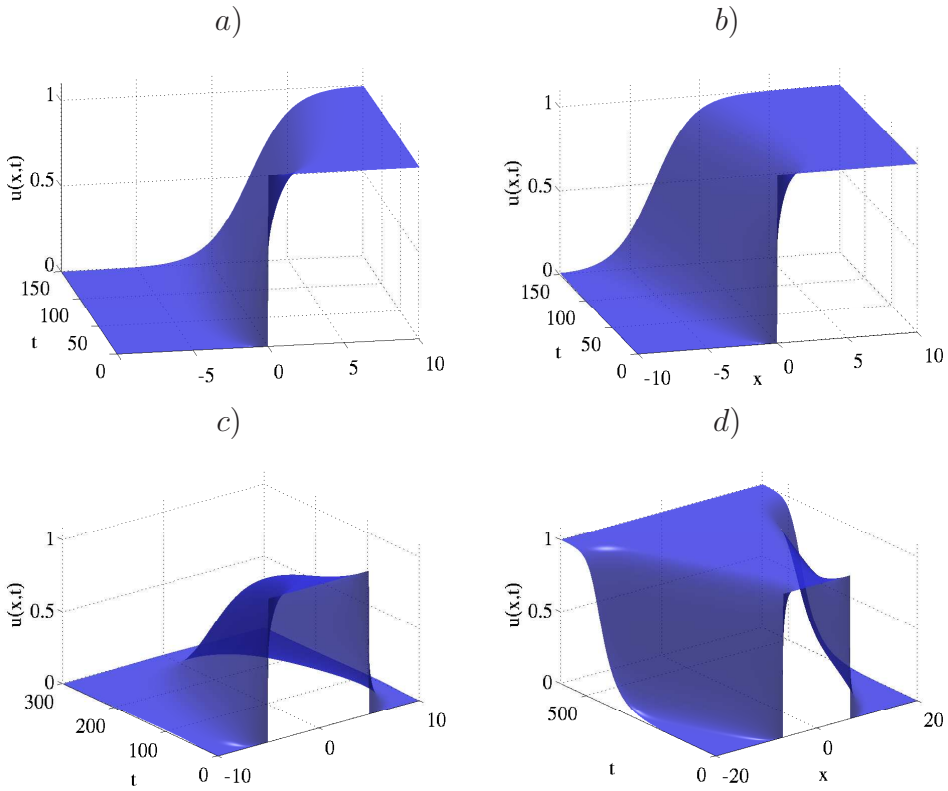


Figure 3.10: Numerical solution of Eq. (3.20), calculated in four different cases. a) a moving front, $\beta = 0.8$; b) a moving front, $\beta = 0.1$; c) collision of two fronts, $\beta = 0.8$; d) scattering of two fronts. $\beta = 0.1$.

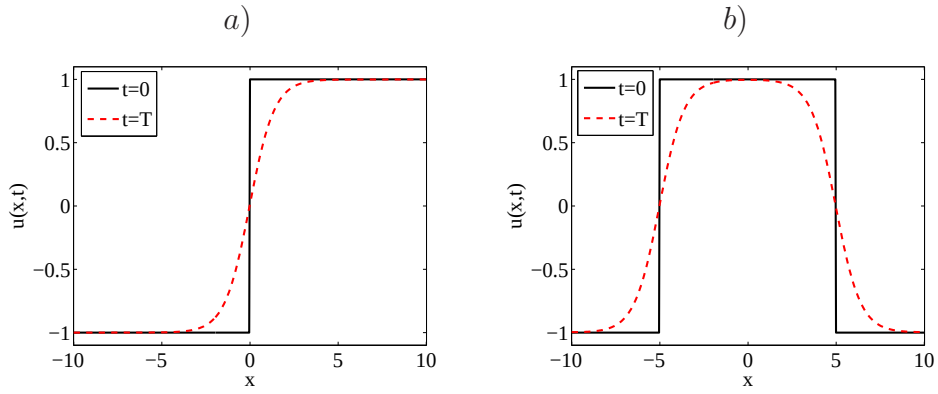


Figure 3.11: Numerical solution of Eq. (3.20). a) Stable stationary front. b) A stable stationary pulse.

| | |
|---|---|
| `Space interval` | $L = 10$ |
| `Space discretization step` | $\triangle x = 0.04$ |
| `Time discretization step` | $\triangle t = 0.05$ |
| `Amount of time steps` | $T = 100$ |
| `Diffusion coefficient` | $D = 1$ |

Initial distribution:

a) Stationary Front:

$$u(x,0) = \begin{cases} u_-, & \text{for} \quad x \leq 0 \\ u_+, & \text{for} \quad x > 0 \end{cases}$$

b) Stationary Pulse:

$$u(x,0) = \begin{cases} u_-, & \text{for} \quad x \in [-L,\, -L/4] \\ u_+, & \text{for} \quad x \in (-L/4, L/4) \\ u_-, & \text{for} \quad x \in [L/4,\, L] \end{cases}$$

Solutions for both cases are shown on Fig. (3.3.3)

## 3.3 Diffusion equation in 2D

Let us consider the solution of the diffusion equation in two dimensions

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right), \tag{3.21}$$

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 $x$- 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 $x$-direction, we discretize on the uniform grid $x_i = x_0 + i\triangle x$, $i = 0, M + 1$, $\triangle x = (b_x - a_x)/(M + 1)$, whereas in the $y$-direction we also consider the uniform grid $y_j = y_0 + j\triangle y$, $i = 0, N + 1$, $\triangle y = (b_y - a_y)/(N + 1)$.

### 3.3.1 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 $\beta = D\triangle t/\triangle y^2$

$$\boxed{u_{ij}^{n+1} = \alpha(u_{i+1j}^n + u_{i-1j}^n) + \beta(u_{ij+1}^n + u_{ij-1}^n) + (1 - 2\alpha - 2\beta)u_{ij}^n.} \tag{3.22}$$

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

$$\alpha + \beta \leq \frac{1}{2} \tag{3.23}$$

This stability condition imposes a limit on the time step:

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

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

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

wich is more restrictive than in the one-dimensional case.

### 3.3.2 BTCS method in 2D

To overcome the stability restriction, we can use an implicit BTCS scheme in the two-dimensional case. The scheme 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

$$\boxed{-\alpha(u_{i+1j}^{n+1}+u_{i-1j}^{n+1})+(1+2\alpha+2\beta)u_{ij}^{n+1}-\beta(u_{ij+1}^{n+1}+u_{ij-1}^{n+1})=u_{ij}^{n}} \qquad (3.24)$$

Let us consider the approximation (3.24) on the $5\times 5$ 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 scheme 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.

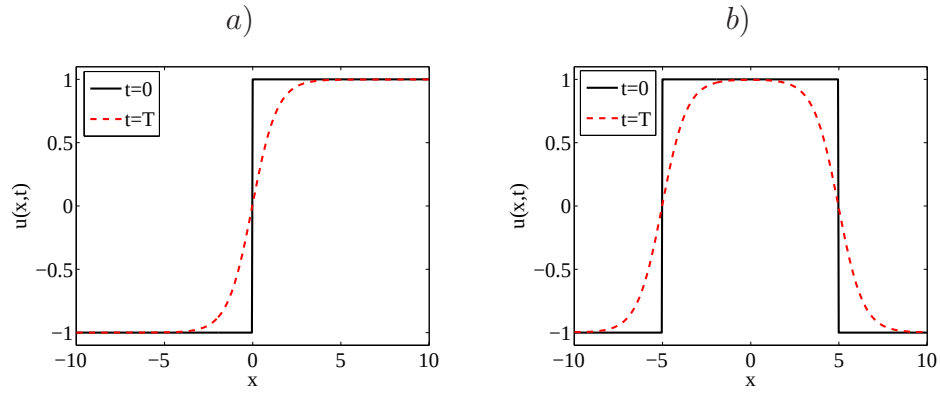


Figure 3.12: Numerical solution of Eq. (3.20). a) Stable stationary front. b) A stable stationary pulse.

### 3.3.3 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. 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:

$$\begin{aligned}-\alpha u_{i+1j}^{n+1/2}+(1+2\alpha)u_{ij}^{n+1/2}-\alpha u_{i-1j}^{n+1/2}&=\beta u_{ij+1}^{n}+(1-2\beta)u_{ij}^{n}+\beta u_{ij-1}^{n}\\ -\beta u_{ij+1}^{n+1}+(1+2\beta)u_{ij}^{n+1}-\beta u_{ij-1}^{n+1}&=\alpha u_{i+1j}^{n+1/2}+(1-2\alpha)u_{ij}^{n+1/2}+\alpha u_{i+1j}^{n+1/2}\end{aligned}$$

Instead of five-band matrix in BTCS method, 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 (however, the ADI in 3D is conditional stable only).

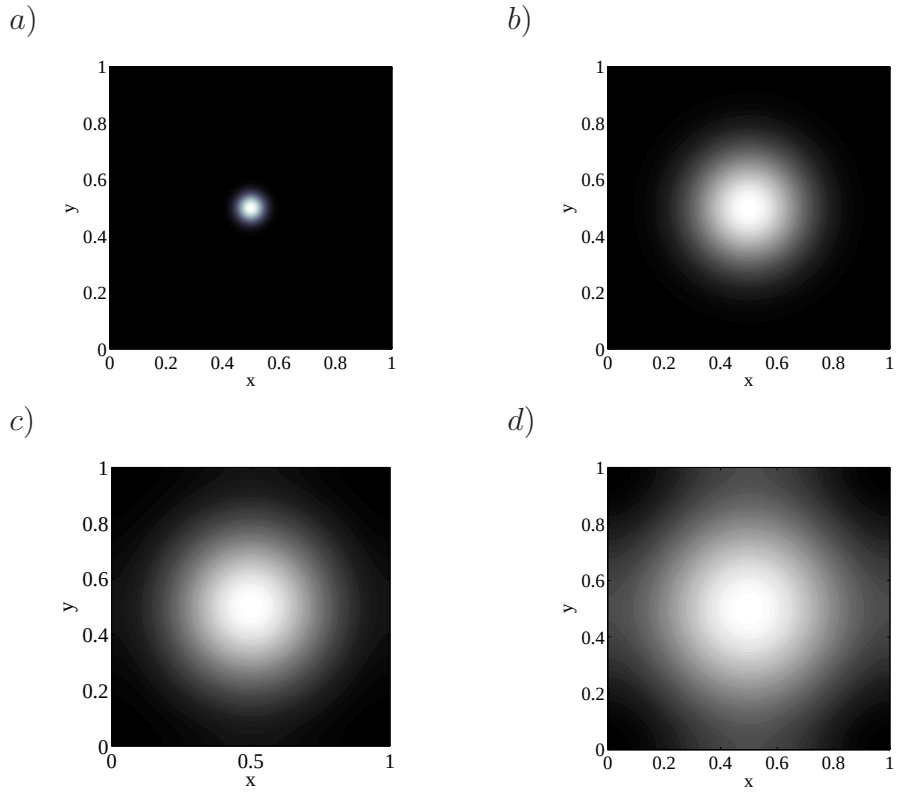


Figure 3.13: Numerical solution of the two-dimensional diffusion equation 3.2 four four different times. a) t=0; b) t=10; c) t=20; d) t=40.

### 3.3.4 Examples

Use the ADI method to solve the one-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 $u_r(0, t) = u_r(L, t) = 0$.

| | |
|---|---|
| `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. (3.3.4).

### 3.3.5 Two-component RD systems: Turing bifurcation

A Turing instability (or bifurcation) involves the destabilization of a homogeneus solution to form a static periodic spatial pattern (Turing pattern), whose wavelength depends on the local reaction kinetic parameters, diffusion coefficients of the system and is its intrinsic property. The hypothesis that just a difference in diffusion constants of components could be enough to destabilize the homogeneous solution was put forward by *A. M. Turing* in 1952 [**?**]. By studying the problem of biological morphogenesis he showed that a reaction-diffusion system with a different diffusion constants can autonomously produce stationary spatial patterns.

We start our analysis of Turing instability from by considering a reaction-diffusion system in general form, restricting ourself first to the case of two components, i.e.,

$$\partial_t \mathbf{u} = \mathbf{D}\nabla^2 \mathbf{u} + \mathbf{R}(\mathbf{u}) \tag{3.25}$$

where $\mathbf{u} = \mathbf{u}(\mathbf{r}, \mathbf{t}) = (u, v)^T$ is a vector of concentration variables, $\mathbf{R}(\mathbf{u}) = (f(u, v), g(u, v))^T$ describes as before a local reaction kinetics and the Laplace operator $\nabla^2$ acts on the vector $\mathbf{u}$ componentwise. $\mathbf{D}$ denotes a diagonal diffusion coefficient matrix,

$$\mathbf{D} = \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix}.$$

Note that we suppose the system 3.25 to be isotropic and homogeneous, so $\mathbf{D}$ is a scalar matrix, independent on coordinates.

Let $\mathbf{u_0} = (u_0, v_0)^T$ be a homogeneous solution (or steady-state solution) of the system (3.25), i.e. $f(u_0, v_0) = g(u_0, v_0) = 0$. Suppose that this solution is stable in absence of diffusion, namely the real parts of all eigenvalues of the Jacobi matrix

$$\mathbf{A} = (\partial \mathbf{R}/\partial \mathbf{u})_{\mathbf{u}=\mathbf{u_0}} = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}$$

describing the local dynamics of the system (3.25) are less that zero. For the case of a 2×2 matrix this is equivalent to the simple well-known condition for the trace and the determinant of the matrix $\mathbf{A}$ (Vite's formula), namely

$$\begin{aligned} \mathrm{Sp}(\mathbf{A}) &= \lambda_1 + \lambda_2 = f_u + g_v < 0 \\ \det(\mathbf{A}) &= \lambda_1 \lambda_2 = = f_u g_v - f_v g_u > 0. \end{aligned} \tag{3.26}$$

Keeping Eq. (3.26) in mind let us see if the presence of diffusion term can change the stability of $\mathbf{u_0}$. To this end, consider a small perturbation $\tilde{\mathbf{u}}$, i.e. $\mathbf{u} = \mathbf{u_0} + \tilde{\mathbf{u}}$ and the corresponding linear equation for it:

$$\partial_t \tilde{\mathbf{u}} = \mathbf{D}\nabla^2 \tilde{\mathbf{u}} + \mathbf{A}\tilde{\mathbf{u}}. \tag{3.27}$$

After decomposition $\tilde{\mathbf{u}}$ into modes $\tilde{\mathbf{u}} \sim \mathbf{a_k} e^{ikr}$ we get the equation

$$\dot{\mathbf{a}}_\mathbf{k} = \mathbf{B}\mathbf{a}_\mathbf{k}, \tag{3.28}$$

where $\mathbf{B} = \mathbf{A} - k^2\mathbf{D}$.

As we have previously mentioned the stability conditions for the system (3.28) with a 2×2 matrix $\mathbf{B}$ can be written as:

$$\begin{aligned} \mathrm{Sp}(\mathbf{B}) < 0 \quad \forall k \\ \det(\mathbf{B}) > 0 \quad \forall k, \end{aligned} \tag{3.29}$$

where

$$\mathrm{Sp}(\mathbf{B}) = -(D_u + D_v)k^2 + \mathrm{Sp}(\mathbf{A}), \tag{3.30}$$

$$\det(\mathbf{B}) = D_u D_v k^4 - (D_u g_v + D_v f_u)k^2 + \det(\mathbf{A}). \tag{3.31}$$

Notice, that for $k = 0$ the conditions (3.29) are equivalent to the stability criterion (3.26) for the local dynamics. In particular this implies that $\mathrm{Sp}(\mathbf{B}) < 0$ for all $k$ (see gray curve in Fig. 3.3.5 for illustration), so the instability of the homogeneous solution can occur only due to violation of the second condition (3.29), that is, $\det(\mathbf{B})$ should be equal to zero for some $k$. It means that the instability occur at the point where the equation $\det(\mathbf{B}) = 0$ has a multiple root. To find it we can simply calculate a minimum of the function $T(k) = \det(\mathbf{B})$.

$$T'(k) = 4D_u D_v k^3 - 2(D_u g_v + D_v f_u)k = 0 \quad \Rightarrow \quad k^2 = \frac{1}{2}\left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right)$$

From the last equation can be seen that the described above situation is possible if

$$D_u g_v + D_v f_u > 0 \tag{3.32}$$

In this case the critical wavenumber is

$$k_c = \sqrt{\frac{1}{2}\left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right)} \tag{3.33}$$

and instability occurs on condition that

$$T(k_c) \le 0 \quad \Leftrightarrow \quad k_c^4 = \left(\frac{1}{2}\left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right)\right)^2 > \frac{\det\mathbf{A}}{D_u D_v} \tag{3.34}$$

The instability scenario, described above is illustrated in Fig. 3.3.5, where three different cases of dependence of the function $T(k) = \det(\mathbf{B})$ on the wave

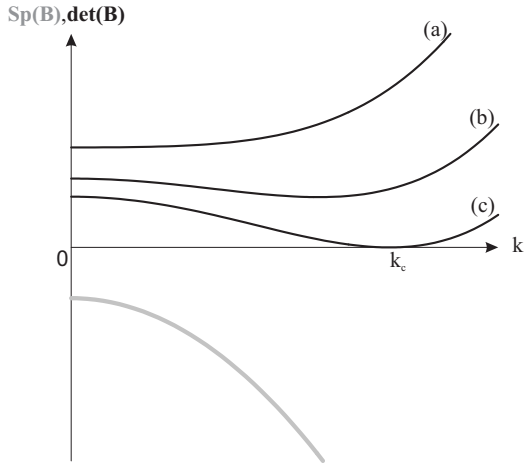


Figure 3.14: Three different cases of dependence of the function $T(k) = \det(\mathbf{B})$ on the wave vector $k$ are presented. (a) the function $T(k)$ has no roots, so the stability of $\mathbf{u_0}$ is not affected as well as in the case (b). $T(k) > 0$ for all $k$, but minimum of this function exists. (c) $T(k) = 0$ for $k = k_c$, indicating the onset of instability.

vector $k$ are presented. In Fig. 3.3.5(a) the function $T(k)$ has no roots, so the stability of $\mathbf{u_0}$ is not affected as well as in the case (b). Here $T(k) > 0$ for all $k$, but minimum of this function exists. Finally, in Fig. 3.3.5(c) $T(k) = 0$ for $k = k_c$, indicating the onset of instability.

Hence, the full system of the conditions for instability of the homogeneous solution $\mathbf{u_0}$ is

$$\boxed{\begin{aligned} f_u + g_v &< 0, \\ f_u g_v - f_v g_u &> 0, \\ D_u g_v + D_v f_u &> 0, \\ \left(\frac{f_u}{D_u} + \frac{g_v}{D_v}\right)^2 &> \frac{4\det\mathbf{A}}{D_u D_v}. \end{aligned}} \tag{3.35}$$

While the conditions for the onset of a Turing bifurcation are rather simple, the determination of the nature of the pattern that is selected is a more difficult problem since beyond the bifurcation point a finite band of wavenumbers is unstable. Pattern selection is usually approached by studying *amplitude equations* that are valid near the onset of the instability. To determine which modes are selected, modes and their complex conjugates are usually treated in pairs so that the concentration field, expanded about the

homogeneous solution, reads

$$\mathbf{u}(\mathbf{r},t) = \mathbf{u_0} + \sum_{j=1}^{n} \big(A_j(t) e^{i\mathbf{k_j r}} + c.c\big),$$

where $\mathbf{k_j}$ are different wavevectors such that $|\mathbf{k_j}| = k_c$. In one dimensional space the situation is rather simple, as result of the instability is represented by a periodic in space structure. In two space dimension this form leads to *stripes* for $n = 1$, *rhombi* (or *squares*) for $n = 2$ and *hexagons* for $n = 3$. The pattern and wavelength that is selected depends on coefficients in the nonlinear amplitude equation for the complex amplitude $A_j$, but some conclusions about selected pattern can be made using, e.g., symmetry arguments. In particular, in the case of hexagonal pattern, in which three wave vectors are mutually situated at an angle of $2\pi/3$, i.e., $\mathbf{k_1} + \mathbf{k_2} + \mathbf{k_3} = 0$, the absence of inversion symmetry ($\mathbf{u} \mapsto -\mathbf{u}$) leads to additional quadratic nonlinearity in the amplitude equation. The latter, in its turn, ends in a fact, that hexagonal pattern has the maximum growth rate near the threshold and is therefor preferred (for details see [**?**]).

The general procedure in details for the derivation of such amplitude equations based on mode projection techniques can be found in [**?**]. Another approach, using multi scale expansion was evolved in [**?**].

### Brusselator model

The Brusselator model is a classical reactiondiffusion system, proposed by I. Prigogine and co-workers in Brussels in 1971. The model describes some chemical reaction with two components

$$u_t = D_u \triangle u + a - (b+1)u + u^2 v, \tag{3.36}$$
$$v_t = D_v \triangle v + bu - u^2 v. \tag{3.37}$$

Here $u = u(x,y,t)$, $v = v(x,y,t)$, $a$, $b$ are posotive constants. The steady state solution is

$$u_0 = a, \quad v_0 = \frac{b}{a}.$$

For the system (3.36) the matrices $\mathbf{D}, \mathbf{A}$ and $\mathbf{B}$ are given by

$$\mathbf{D} = \begin{pmatrix} D_u & 0 \\ 0 & D_v \end{pmatrix}, \quad \mathbf{A} = \begin{pmatrix} b-1 & a^2 \\ -b & -a^2 \end{pmatrix},$$

and

$$\mathbf{B} = \begin{pmatrix} b - 1 - D_u k^2 & a^2 \\ -b & -D_v k^2 - a^2 \end{pmatrix}.$$

Suppose that the system (3.36) is local stable, i.e.,

$$\begin{aligned}\mathrm{Sp}(\mathbf{A}) &= b - 1 - a^2 < 0,\\ \mathrm{Det}(\mathbf{A}) &= -(b-1)a^2 + a^2 b = a^2 > 0.\end{aligned}$$

Note that the violation of the first condition above leads to tthe Hopf bifurcation, i.e., the onset of Hopf instability is

$$\boxed{\mathrm{Sp}(\mathbf{A}) \geq 0 \Leftrightarrow b \geq b_H = 1 + a^2.}$$

The critical wavenumber is

$$k_c = \sqrt{\frac{1}{2}\left(\frac{b-1}{D_u} - \frac{a^2}{D_v}\right)}$$

The existence of $k_c$ is equivalent to the following condition

$$b > 1 + \frac{D_u}{D_v}a^2 + 1 \Rightarrow \frac{D_u}{D_v} < 1.$$

The instability occurs, if

$$\mathrm{Det}(\mathbf{B}(k_c)) \leq 0 \Leftrightarrow b > b_T = \left(1 + a\sqrt{\frac{D_u}{D_v}}\right)^2.$$

Hence, the conditions (3.35) for the system (3.36) takes the form

$$\boxed{\begin{array}{l} b < b_H = 1 + a^2,\\ b > b_T = \left(1 + a\sqrt{\dfrac{D_u}{D_v}}\right)^2,\\ \dfrac{D_u}{D_v} < 1. \end{array}} \tag{3.38}$$

On Fig. (3.3.5) both functions $b_H$, $b_T$ are shown. The thresholds of these two instabilities coincide at codimensional-two Turing-Hopf point $b_H = b_T$ ($\sigma = D_u/D_v$)

$$a_c = \frac{2\sqrt{\sigma}}{1-\sigma}.$$

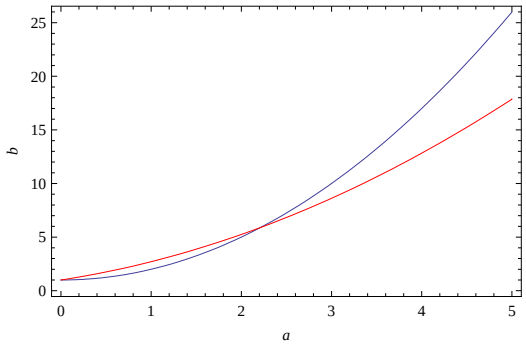


Figure 3.15: Bifurcation diagram in $(a, b)$ parameter space, indicating the onset of Hopf (blue line) and Turing (red line) instabilities. Here $D_u = 5$, $D_v = 12$

# Chapter 4

# Elliptic PDE's

The basic example of an elliptic partial differential equation is *Laplace's equation*

$$\nabla^2 u(\mathbf{r}) = 0, \tag{4.1}$$

where $u(\mathbf{r})$ is a scalar function and $\mathbf{r} \in \Omega \subseteq \mathbb{R}^2, \mathbb{R}^3$. Laplace's equation is a special case of *the Helmholtz differential equation*

$$\nabla^2 u(\mathbf{r}) + k^2 u(\mathbf{r}) = 0 \tag{4.2}$$

with $k = 0$ or *Poisson's equation*

$$\nabla^2 u(\mathbf{r}) = f(\mathbf{r}), \tag{4.3}$$

where $u(\mathbf{r})$ is usually some sort of potential and $f(\mathbf{r})$ a real source term.

In general all these equations are subject to boundary conditions at the outer boundary of $\Omega$. No initial conditions, such as we would expect, e.g., for the wave or heat equations, are typically given.

## 4.1 Poisson Equation in 1D

### 4.1.1 Dirichlet boundary conditions

As a simple test case, we start to consider the solution of Poisson's equation in one dimension

$$\frac{\partial^2 u(x)}{\partial x^2} = f(x) \tag{4.4}$$

for $x \in [a, b]$. Suppose that Eq. (4.4) is the subject to the Dirichlet boundary conditions $u(a) = u_a$ and $u(b) = u_b$. If we define a grid on the intervall $[a, b]$ one can rewrite Eq. (4.4) using a second-order, central difference scheme

$$u_{i-1} - 2u_i + u_{i+1} = \triangle x^2 f_i, \qquad i = 1, \ldots, M,$$

where $f_i = f(x_i)$. Futhermore, $u_0 = u_a$, $u_{M+1} = u_b$. This system of algebraic equations can be rewritten in a matrix form

$$\begin{pmatrix} -2 & 1 & 0 & \dots & \dots & 0 \\ 1 & -2 & 1 & \dots & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & 1 \\ 0 & \dots & \dots & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \cdot \\ \cdot \\ u_M \end{pmatrix} = \begin{pmatrix} \triangle x^2 f_1 - u_a \\ \triangle x^2 f_2 \\ \cdot \\ \cdot \\ \triangle x^2 f_1 - u_b \end{pmatrix}. \tag{4.5}$$

with a tridiagonal matrix $A$. The formal solution

$$\mathbf{u} = A^{-1}\mathbf{b}$$

can be found ba use of, e.g., TDMA.

### 4.1.2 Mixed boundary conditions

Let us now consider the more general set of mixed boundary conditions:

$$\alpha_l u + \beta_l \frac{\partial u}{\partial x} = \gamma_l \quad \text{for} \quad x = a$$
$$\alpha_r u + \beta_r \frac{\partial u}{\partial x} = \gamma_r \quad \text{for} \quad x = b.$$

Here $\alpha_l$, $\alpha_r$, $\beta_l$, $\beta_r$, $\gamma_l$, $\gamma_r$ are known constants. Using the previous notation, the discretized version of boundary conditions in question is ($i = 0$, $i = M + 1$)

$$\alpha_l u_0 + \beta_l \frac{u_1 - u_0}{\triangle x} = \gamma_l,$$
$$\alpha_r u_{M+1} + \beta_r \frac{u_{M+1} - u_M}{\triangle x} = \gamma_r,$$

giving

$$u_0 = \frac{\gamma_l \triangle x - \beta_l u_1}{\triangle x \alpha_l - \beta_l},$$
$$u_{M+1} = \frac{\gamma_r \triangle x + \beta_h u_M}{\triangle x \alpha_r + \beta_r}.$$

Using these expressions the problem can also be reduced to a tridiagonal matrix equation

$$\begin{pmatrix} -2 + b_1 & 1 & 0 & \dots & \dots & 0 \\ 1 & -2 & 1 & \dots & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & 1 \\ 0 & \dots & \dots & 0 & 1 & -2 + b_M \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \cdot \\ \cdot \\ u_M \end{pmatrix} = \begin{pmatrix} \triangle x^2 f_1 - a_1 \\ \triangle x^2 f_2 \\ \cdot \\ \cdot \\ \triangle x^2 f_1 - a_n \end{pmatrix}, \tag{4.6}$$

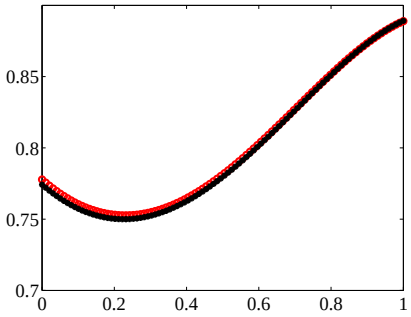


Figure 4.1: Numerical solution of the one-dimensional Poisson equation 4.4.The red line shows the analytic solution, whereas the black one stands for the numerical solution for $M = 100$.

where

$$b_1 = \frac{-\beta_l}{\triangle x \alpha_l - \beta_l}, \quad b_M = \frac{\beta_r}{\triangle x \alpha_r + \beta_r},$$
$$a_1 = \frac{\gamma_l \triangle x}{\triangle x \alpha_l - \beta_l}, \quad a_M = \frac{\gamma_r \triangle x}{\triangle x \alpha_r + \beta_r}.$$

### 4.1.3 Example

Let us now solve 1D Poisson's equation (4.4), with mixed boundary conditions, using the technique discussed above. We are looking for the solution of

$$\frac{\partial^2 u(x)}{\partial x^2} = 1 - 2x^2$$

on the interval $x \in [0, 1]$ with the following boundary conditions

$$u - \frac{\partial u}{\partial x} = 1 \quad \text{for} \quad x = 0$$
$$u + \frac{\partial u}{\partial x} = 1 \quad \text{for} \quad x = 1.$$

The analytical solution is

$$u(x) = \frac{-2x}{9} + \frac{7}{9} + \frac{x^2}{2} - \frac{x^4}{6},$$

Figure shows a comparison between the analytic and finite difference solutions for $M = 100$.

## 4.2 Two-dimensional problems

### 4.2.1 Laplace's equation in 2D

Let us consider the Laplace's equation (4.1)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

on the rectangle $R = [0,\, a] \times [0,\, b]$. Assume, that we define also a $M \times N$grid on $R$ with the grid step $h$. Let us also consider the central approximation for the second derivatives

$$\boxed{u_{i+1j} + u_{i-1j} + u_{ij+1} + u_{ij-1} - 4u_{ij} = 0},$$

which is known as *the five-point difference formula* for Eq. (4.1).

#### Dirichlet boundary conditions

Suppose that the values $u(x, y)$ are known at the following boundary grid points:

$$\begin{aligned}
u(x_1, y_j) &= u_{1j}, \quad j = 2, \ldots, M-1, \quad \text{(on the left)},\\
u(x_i, y_1) &= u_{i1}, \quad i = 2, \ldots, N-1, \quad \text{(on the bottom)},\\
u(x_N, y_j) &= u_{Nj}, \quad j = 2, \ldots, M-1, \quad \text{(on the right)},\\
u(x_i, y_M) &= u_{iM}, \quad i = 2, \ldots, N-1, \quad \text{(on the top)}.
\end{aligned}$$

Applying the five-point formula at each of interior points of $R$ we get a linear system of $N-2 \times M-2$ equations. For example, if we consider a special case $M = N = 5$ the system can be written as

$$\left(\begin{array}{ccc|ccc|ccc}
-4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\
1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0\\
0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0\\
\hline
1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0\\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0\\
0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1\\
\hline
0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0\\
0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4
\end{array}\right)
\begin{pmatrix} u_{22}\\ u_{23}\\ u_{24}\\ \hline u_{32}\\ u_{33}\\ u_{34}\\ \hline u_{42}\\ u_{43}\\ u_{44} \end{pmatrix}
=
\begin{pmatrix} -u_{12} - u_{21}\\ -u_{13}\\ -u_{14} - u_{25}\\ \hline -u_{31}\\ 0\\ -u_{35}\\ \hline -u_{52} - u_{41}\\ -u_{53}\\ -u_{54} - u_{45} \end{pmatrix}$$

On can see, that the matrix of the system is a five-band matrix. To solve the system in question a Gauss-illimination-like-algorithm can be applied. As an alternative iterative or spectral methods can be used.

### 4.2.2 Iterative methods

The term "iterative method" refers to a wide range of techniques that use successive approximations to obtain more accurate solutions to a linear system

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

at each step. Iterative methods that can be expressed in the simple form

$$\mathbf{u}^k = B\mathbf{u}^{k-1} + c$$

(where neither nor depend upon the iteration count ) are called stationary iterative methods. In this section, we consider three main stationary iterative methods: the Jacobi method, the Gauss-Seidel method and the Successive Overrelaxation (SOR) method.

**The Jacobi method**

**The Gauss-Seidel method**

**The SOR method**

# .1 Tridiagonal matrix algorithm (TDMA)

The tridiagonal matrix algorithm (TDMA), also known als *Thomas algorithm*, is a simplified form of Gaussian elimination that can be used to solve tridiagonal system of equations

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = y_i, \qquad i = 1, \ldots n, \tag{7}$$

or, in matrix form ( $a_1 = 0$, $c_n = 0$)

$$\begin{pmatrix} b_1 & c_1 & 0 & \ldots & \ldots & 0 \\ a_2 & b_2 & c_2 & \ldots & \ldots & 0 \\ 0 & a_3 & b_3 & c_3 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & c_{n-1} \\ 0 & \ldots & \ldots & 0 & a_n & b_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ y_n \end{pmatrix}$$

The TDMA is based on the Gaussian elimination procedure and consist of two parts: a forward elimination phase and a backward substitution phase. Let us consider the system (7) for $i = 1 \ldots n$ and consider modifying the second equation (for $i = 2$) with the first equation ($i = 1$) as follows:

$$\mathrm{Eq}_{i=2} \cdot b_1 - \mathrm{Eq}_{i=1} \cdot a_2$$

which relults in

$$(b_1 b_2 - c_1 a_2) x_2 + c_2 b_1 x_3 = b_1 y_2 - a_2 y_1.$$

The effect is that $x_1$ has been eliminated from the second equation. In the same manner one can eliminate $x_2$, using the modified second equation and the third one (for $i = 3$):

$$(b_1 b_2 - c_1 a_2)\mathrm{Eq}_{i=3} - a_3(\text{mod. } \mathrm{Eq}_{i=2}),$$

which would give

$$(b_3(b_1 b_2 - c_1 a_2) - c_2 b_1 a_3) x_3 + c_3(b_1 b_2 - c_1 a_2) x_4 = y_3(b_1 b_2 - c_1 a_2) - (y_2 b_1 - y_1 a_2) a_3$$

If the procedure is repeated until the n'th equation, the last equation will involve the unknown function $x_n$ only. This function can be then used to solve the modified equation for $i = n - 1$ and so on, until all unknown $x_i$ are found (backward substitution phase). That is, we are looking for a backward ansatz of the form:

$$x_{i-1} = \gamma_i x_i + \beta_i. \tag{8}$$

If we put the last ansatz in the Eq. (7) and solve the resulting equation with respect to $x_i$, the following relation can be obtained:

$$x_i = \frac{-c_i}{a_i\gamma_i + b_i}x_{i+1} + \frac{y_i - a_i\beta_i}{a_i\gamma_i + b_i} \tag{9}$$

This relation possesses the same form as Eq. (8) if we identify

$$\boxed{\gamma_{i+1} = \frac{-c_i}{a_i\gamma_i + b_i}, \qquad \beta_{i+1} = \frac{y_i - a_i\beta_i}{a_i\gamma_i + b_i}}. \tag{10}$$

Equation (10) involves the recursion formula for the coefficients $\gamma_i$ and $\beta_i$ for $i = 2, \ldots, n-1$. The missing values $\gamma_1$ and $\beta_1$ can be derived from the first $(i = 1)$ equation (7):

$$x_1 = \frac{y_1}{b_1} - \frac{c_1}{b_1}x_2 \Rightarrow \gamma_2 = -\frac{c_1}{b_1},\ \beta_2 = \frac{1}{b_1} \Rightarrow \boxed{\gamma_1 = \beta_1 = 0.}$$

The last what we need is the value of the function $x_n$ for the first backward substitution. We can obtain if we put the ansatz

$$x_{n-1} = \gamma x_n + \beta_n$$

into the last $(i = n)$ equation (7):

$$a_n(\gamma x_n + \beta_n) + b_n x_n = y_n,$$

yielding

$$x_n = \frac{y_n - a_n\beta_n}{a_n\gamma_n + b_n}.$$

One can get this value directly from Eq. (8), if one formal puts

$$x_{n+1} = 0.$$

Altogether, the TDMA can be written as:

1. `Set` $\gamma_1 = \beta_1 = 0$;

2. `Evaluate for` $i = 1, \ldots, n-1$

$$\gamma_{i+1} = \frac{-c_i}{a_i\gamma_i + b_i}, \qquad \beta_{i+1} = \frac{y_i - a_i\beta_i}{a_i\gamma_i + b_i};$$

3. `Set` $x_{n+1} = 0$;

4. `Find for` $i = n+1, \ldots, 2$

$$x_{i-1} = \gamma_i x_i + \beta_i.$$

The algorithm admits $\mathcal{O}(n)$ operations instead of $\mathcal{O}(n^3)$ required by Gaussian elimination.

### Limitation

The TDMA is only applicable to matrices that are diagonally dominant, i.e.,

$$|b_i| > |a_i| + |c_i|, \qquad i = 1, \ldots, n.$$

### Variants

If the PDE in question involves periodic boundary conditions, the resulting tridiagonal system is slightly different from the system (7), namely

$$\begin{pmatrix} b_1 & c_1 & 0 & \ldots & \ldots & a_1 \\ a_2 & b_2 & c_2 & \ldots & \ldots & 0 \\ 0 & a_3 & b_3 & c_3 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & c_{n-1} \\ c_n & \ldots & \ldots & 0 & a_n & b_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ y_n \end{pmatrix} \Leftrightarrow A\mathbf{x} = \mathbf{y}. \tag{11}$$

In this case one can make use of the *Sherman-Morrison formula* to avoid additional operations and still use TDMA.

Let us consider two $n \times n$ matrices $A$ and $B$ that are related by

$$A = B - \mathbf{u}\mathbf{v}^T,$$

where $\mathbf{u}$ and $\mathbf{v}$ are $n$-vectors, $A$ is a matrix defined by (11) and $B$ is some tridiagonal matrix. Then, if $B^{-1} \neq 0$ and the scalar $\mathbf{v}^T B^{-1} u \neq 1$, $A^{-1}$ exists and can be found using Sherman-Morrison formula:

$$A^{-1} = B^{-1} + \frac{B^{-1}\mathbf{u}\mathbf{v}^T B^{-1}}{1 - \mathbf{v}^T B^{-1}\mathbf{u}} \tag{12}$$

Applying the relation above we note that

$$\mathbf{x} = A^{-1}\mathbf{b} = B^{-1}\mathbf{b} + \frac{B^{-1}\mathbf{u}\mathbf{v}^T B^{-1} b}{1 - \mathbf{v}^T B^{-1}\mathbf{u}} = B^{-1}b + \frac{\mathbf{v}^T B^{-1} b}{1 - \mathbf{v}^T B^{-1}\mathbf{u}} B^{-1}\mathbf{u}.$$

Thus, the system (11) can be solved as follows:

1. Solve (TDMA)

$$B\mathbf{x_1} = b, \qquad B\mathbf{x_2} = \mathbf{u};$$

2. Set

$$\beta := \frac{\mathbf{v}^T B^{-1} b}{1 - \mathbf{v}^T B^{-1}\mathbf{u}} = \frac{\mathbf{v}^T \mathbf{x_1}}{1 - \mathbf{v}^T \mathbf{x_2}};$$

3. Evaluate

$$\mathbf{x} = \mathbf{x_1} + \beta \mathbf{x_2}.$$

In the case of system (11) the matrix $B$ and vectors $\mathbf{u}$ and $\mathbf{v}$ can be choosen as:

$$B = \begin{pmatrix} b_1 - 1 & c_1 & 0 & \dots & \dots & 0 \\ a_2 & b_2 & c_2 & \dots & \dots & 0 \\ 0 & a_3 & b_3 & c_3 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & c_{n-1} \\ 0 & \dots & \dots & 0 & a_n & b_n - a_1 c_n \end{pmatrix}, \mathbf{u} = \begin{pmatrix} b_1 \\ 0 \\ \cdot \\ 0 \\ c_n b_1 \end{pmatrix}, \mathbf{v} = \begin{pmatrix} -1/b_1 \\ 0 \\ \cdot \\ 0 \\ -a_1/b_1 \end{pmatrix}.$$