# Computer simulations

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# **Revision History**

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# 1 Introduction

## 1.1 Objectives

The main goal of this lab is to solve physical problems with the help of computer to handle simulations. Computer simulations in the sense of this lab are programs on a computer, the purpose of which is to make a quantitative model of some aspect of a physical system. The computer is used because in many questions the number of arithmetic operations required to get an answer from a model can be enormous. It is possible to already have a table in a spreadsheet program to understand simulation. On the other hand, the numerical models we are considering here are in the area between the numerical calculation of an integral (numerical quadrature), the simulation of tomorrow's weather, an avalanche, or the force, pull and pressure distribution of the heart muscle during blood pumping. Because this lab will also appeal to people with little or no computer experience, it is a further goal to enable entry into the world of computer simulation. Many problems from science can be mathematically referred to as differential equations. Thereby, between the ordinary and the partial differential equations is to differentiate. The former only contain derivatives with respective to one variable, in the latter there are derivatives with respective to two or more variables. Compared to an ordinary differential equation, solving a partial differential equation can be immensely cumbersome. The more common solution methods are limited by the numerical treatment. However, the task here is to also solve a partial differential equation with numerical methods. For example, in the case of partial differential equations, care must be taken that the method used converges at all to the desired solution. Unwanted side effects can be oscillations of the numerical solution, which are caused by the method alone and are not of a physical nature. Another problem with numerical solution methods can be the appearance of negative values for quantities that cannot be negative for physical reasons, for examples, concentrations or densities. In addition, considerable effort goes into constructing a method for a given problem, which obey physical conservation laws (e.g. energy, momentum).

#### 1.2 Motivation

Numerical modeling in today's research is an increasingly important topic. This has to do with the collapse in prices of computers which have become very inexpensive, and the growing capacity of computers that allows simulating ever more complex relationships, which are not feasible in experiments or lead to great costs. For example, you find that crash tests at vehicle manufacturers are no longer just in reality, but in some cases purely computer models that try to map the physics of a collision. Another example is the food industry, where numerical models are used to investigate the time-dependent consistency of artificial foods during the chewing movement.

#### 1.3 Question of accuracy

An important point is that the results of a simulation need to be critically assessed, because it is tempting to blindly trust the results of a computer model. But the statements of a computer program are credible, it is often a long way off. Sources of error and discrepancies from reality can creep in:

- Insufficient representation of the physics in the model. For example, it is necessary but not always easy to take into account all terms of the same order in a series expansion.
- an unfavorable numerical method. For example, a method can be used for some parameter values that ensures convergence to the solution, but for other parameter values they do not converge.
- Errors in the program code, errors that are not due to insufficient consideration in physics or mathematics, but for example through demonstration error, or because an index starts at 1 instead of 0, etc.

The first step in recognizing sources of error is to develop a distrust of each other your own results. The second step then is to run tests. In the best case, one knows the analytical solution with which the numerical result can be compared. However, in this situation no numerical simulation is necessary. After all, it is conceivable that the analytical solution for special cases is known. Another way is to carry out the simulation with varying resolution. Since the solution must not depend on the resolution, this can be formulated positively estimate the accuracy of the results. The negative case occurs when the results are below changes in resolution differ too much from the original values, in other words, any result can be obtained. In this case, it is worthwhile to look for mistakes. The third way is to compare the results with an independent model, which may be developed for a special case with little effort. Fourth, it is useful to physically interpret the results. Even if no closed analytical statements are available, we can can often check the order of magnitude of the results, for example time constants or typical speeds can be estimated and compared with the simulation. In addition, it is often possible to check whether the results are qualitatively

meaningful. For example, when simulating an ideal gas, the temperature will rise as the pressure increases and the volume is kept constant.

#### 1.4 Tasks

One of the following physical tasks (sections 2 to 4) must be selected and completed. The workload of the various tasks is intentionally different, in order to accommodate both people with and without experience with computers and programs. Choose an appealing task. The physical background in each proposed problem is kept simple to focus on the computational task.

# 2 Traffic simulation

#### 2.1 Introduction

The simulation of road traffic is an application of increasing importance. Possible applications are, for example, the forecast of traffic jams analogous to weather predictions or the optimization of the layout of roads based on traffic flow criteria. Two approaches are used today to simulate traffic. One is based on that the traffic flow can be understood as a fluid and with hydrodynamic equations. The second approach is the application of cellular automata. Within a road, for example the lane of a motorway, is divided into equidistant cells. A cell is either occupied by a vehicle or it is empty. With each discrete time step, the vehicles are moved forward by a whole number of cells. This number is given by the current vehicle speed, which is dependent, for example on the number of free cells in the direction of travel. A more precise and easily comprehensible descriptions are given in, for example, Schreckenberger et al. (1996) and Chowdhury et al. (2000).

#### 2.2 Tasks

Program a cellular automaton to control the flow of traffic in a ring-shaped, single lane motorway. Examine congestion, the so-called fundamental diagram (traffic flow as a function of vehicle density), the distribution of the distance between two neighboring vehicles, etc. Further investigations are (i) the simulation of a two-lane highway with overtaking maneuvers, and (ii) the simulation of a two-dimensional closed road network with traffic lights or other right of way regulations.

# 3 One-dimensional heat conduction

#### 3.1 Task

We consider the one-dimensional temperature field (the temperature profile) in the top 10-20 m of the ground, which is due to the irradiation of the sun in daily and seasonal rhythm and is time-dependent.

- Preparation: Derive an analytical, time-dependent expression for the zenith angle at which the sun shines on a horizontal surface at a given geographical position. The daily and the annual apparent movement of the sun must be taken into account. At time t = 0, the sun is vertically above the equator, and at the given position is noon, 12 o'clock solar time.
- Write a program that shows the development of the temperature profile over time under the influence of solar radiation and the thermal radiation of the simulated Earth's surface. The radiation is given by  $\epsilon \sigma T^4$ , where  $\epsilon$  is the emissions coefficient in the infrared,  $\sigma$  is the Stefan-Boltzmann constant, and T is the temperature at the surface. We assume that the visible surface has an albedo  $0 \le a \le 1$ , which means that only the portion 1-a of the irradiated sunlight is absorbed. The influence of the atmosphere on the flow of radiation energy is neglected. Chapter 6 in Gershenfeld (2000) can be of help. Use different numerical methods (explicit and implicit) and compare, and write out the the advantages and disadvantages of each technique (see also Appendix A). Present the results graphically in a suitable form. While the program is running, no graphic has to be generated.
- Compare the results you get when the sun moves on the limited daily exercise, with the analytical solution. This is derived in the Section 3.3. Discuss the differences.

## 3.2 Derivation of the one-dimensional heat conduction equation

We consider the part of the earth that is of interest to us as a homogeneous, rigid body with constant density. That means that firstly the transport of thermal energy only comes about due to heat conduction. Convection currents and energy transport in the form of radiation, however, are neglected. Next are the material parameters, which describe the heat conduction, not dependent on the depth z. Also we do not see the temperature distribution over the entire surface of the globe, but only in a local environment. This is small enough that all relevant variables are only dependent on the time and depth, so that there is no temperature gradient in the horizontal direction and no heat flow.

#### 3.2.1 Flow of thermal energy: the heat flow

In the time interval  $\Delta t$  may flow through the cross-sectional area A, the heat Q. The heat flow j is defined by

$$Q = A \Delta t \ j \tag{1}$$

and has the unit  $W/m^2$ .

#### 3.2.2 Change in internal energy

If heat flows into or out of a volume element  $\Delta V = \Delta z A$ , the inner one changes energy of this element. The net flow is due to the difference in heat flow at both ends of the volume element, so follows immediately

$$\Delta U = -[Q(z + \Delta z) - Q(z)] = [j(z + \Delta z) - j(z)]\Delta t A. \tag{2}$$

#### 3.2.3 Change in temperature

The change in the internal energy  $\Delta U$  of a mass element  $\Delta m = \rho A \Delta z$  is with a temperature change  $\Delta T$  connected

$$\Delta U = c\Delta m \Delta T,\tag{3}$$

where  $\rho$  and c are the mass density and the specific heat capacity of the material. We are allowed to write equation

$$c\rho A\Delta z\Delta T = -[j(z + \Delta z) - j(z)]\Delta t A. \tag{4}$$

In the limit  $\Delta z \to 0$  and  $\Delta t \to 0$  this results in

$$c\rho \frac{\partial T}{\partial t} = -\frac{\partial j}{\partial z},\tag{5}$$

the change in temperature over time is due to the spatial inhomogeneity of the heat flow. It is instructive to do this with the mass continuity equation in three spatial dimensions

$$\frac{\partial \rho}{\partial t} + \nabla \mathbf{j}_m = 0 \tag{6}$$

to compare that follows from the conservation of mass. Here,  $\mathbf{j}_m$  is the mass flow that leads to a change in mass density. The factor  $c\rho$  (heat capacity per volume), which appears in (5) but not in (6) only serves to ensure that on one side the equation is the temperature, on the other side, the flow of energy can be written. The formal equality of equations (6) and (5) is not coincidental. Both are based on the fact that a quantity (internal energy or the mass) in a volume only changes when a current (heat flow or mass flow) flows over the edge of the volume. Note: this requirement only applies to internal energy if heat sources, for example, through dissipation or chemical reactions can be excluded. Otherwise the equation can be expanded to include source and sink terms.

## 3.3 Cause of a heat flow

A flow of thermal energy in a body is caused by local temperature natural differences. According to Fourier's approach, the flow is proportional to the temperature

$$j(z,t) = -k\frac{\partial T(z,t)}{\partial z}. (7)$$

The constant of proportionality k is called the coefficient of thermal conductivity and depends on the material. The negative sign expresses that the flow of energy takes place in the direction of the negative gradient.

#### 3.3.1 The heat conduction equation

The combination of equations (5) and (7) gives the heat conduction equation

$$\frac{\partial T}{\partial t} = \frac{k}{c\rho} \frac{\partial^2 T}{\partial z^2} \tag{8}$$

The quotient  $K = k/(c\rho)$  is called the thermal diffusivity. The equation of heat conduction is represented as a partial differential equation. Many problems in physics list equations that have a first derivative with respect to time and a second derivative with respect to position. Often these are transport phenomena. Their characteristic is that, firstly, one gradient of a current causes a change in a quantity over time, which is essentially is the statement of the equation of continuity, and that second is the current through the gradient that the same quantity is triggered. This basic type also occurs in the earlier diffusion example. The diffusion equation for a concentration c of a substance in a liquid (e.g. sugar in water)

$$\frac{\partial c}{\partial t} = D \,\,\partial c \tag{9}$$

with the diffusion coefficient D is formally identical to (8). Other questions that lead to equations of type (9) are the management of electrical charges and the exchange of momentum between liquids with different speed due to viscosity<sup>1</sup>. However, equations of type (8) do not occur when a gradient of a quantity does not trigger current according to the Fourier approach. For example, the planets do not diffuse in the Solar system. The movement of the mass follows here according to the laws of gravity, however, this does not aim to compensate for a density gradient.

# 3.4 Analytical solutions to the heat conduction equation

## 3.4.1 Stationary heat conduction

In order for a solution to a partial differential equation to be defined, the boundary conditions must also be given. The analogue in the usual differential equations is the definition of the initial condition and the (in-)homogeneity. This can be easily understood using the example of the heat conduction equation. We look at a thermally conductive rod. One possibility of specifying the boundary conditions is that the ends of the rod are to be regarded as isolating from the outside. It follows that the total internal energy of the rod remains constant. Internal heat flows ensure that the rod compensates for existing temperature differences and in the entire rod after an intermediate temperature prevails for a long enough time. A second option is both rod ends, for example, in an external heat bath, fixed to a predetermined temperature. Induced internal heat flows are then used to determine the temperature profile inside and the rod adjusts until the temperature is the same everywhere. The difference to the first case is that energy flows into or out of the rod. The commonality of both of the cases is that, after a long enough wait, a thermodynamic equilibrium is reached and macroscopic heat flows no longer take place. A different case in this respect is when the two rod ends on different temperatures are maintained. Now a steady state develops in which the temperature increases linearly along the rod from one end to the other. The stationary temperature distribution remains constant, but in order to maintain it, it flows steadily, with constant heat flow from the hot rod end into the rod, through the rod and finally out at the other end of the rod. In these three cases, the resulting situation can be easily described analytically as long as we only look at the final state, but not at the dynamic development that leads to this. All three cases are characterized by the fact that in the final state, no more temperature changes take place. Formally this means  $\partial T/\partial t = 0$ . By inserting this into the heat conduction equation (8) we get the stationary heat conduction equation

$$\frac{d^2T(z)}{dz^2} = 0\tag{10}$$

Obviously the set of solutions is given by  $T(z) = T_0 + q z$ . From the above, the temperature distributions result immediately from the boundary conditions.

#### 3.4.2 Time-dependent heat conduction

The situation is not just static or stationary when the earth's surface is periodically supplied with energy by the sun and in the when it emits energy at night, the situation is no longer static or stationary. In this case the boundary conditions are functions of time. The energy flows below the surface become time-dependent, and therefore there

<sup>&</sup>lt;sup>1</sup>See, for example, Chapter 18. Signals in the head of the electrodynamics script by H. Leutwyler.

can no longer be a stationary solution. One possibility to solve the heat conduction equation under these boundary conditions is the separation approach

$$T(t,z) = M(z) N(t). (11)$$

So we are looking for solutions that can be represented as the product of two functions, where one function M only depends on the depth z and the function N only on the time t. The motivation for this approach is initially only the experience that it leads to a solution in many cases. As a convention, we specify that the z-axis is oriented downwards, z=0 is the height of the earth's surface, and energy flows are in the direction of the positive z-axis, otherwise negative. The insertion of the separation approach into the heat conduction equation (8) leads us to

$$\frac{\dot{N}(t)}{N(t)} = K \frac{M''(z)}{M(z)} \tag{12}$$

The left side is independent of z, the right side is independent of t, so both sides are constant in t and z. That's why we're allowed to write

$$\frac{\dot{N}(t)}{N(t)} = C = K \frac{M''(z)}{M(z)} \tag{13}$$

with an arbitrary constants C. Solutions for the two functions  $M(t) = M \exp(Ct)$  and  $N(z) = N \exp(\sqrt{C/Kz})$ . From a mathematical point of view, C can be any complex number. However, if C has a vanishing imaginary part, the solution for N becomes unphysical, it explodes with z. It is also reasonable that the time dependency is periodic, because our goal is a periodic supply and release of energy over time looking at the surface of the earth, coming towards us. That is why we limit ourselves to one purely imaginary constant and substitute  $C = i\omega$  with real  $\omega$ . This will be the found solutions

$$M(t) = M \exp(i\omega t)$$
 (14)  
 $N(z) = N \exp\left(\sqrt{i\omega/K}z\right)$ 

The sign of the real part of the root in the exponent must be for physical reasons chosen to be negative so that N(z) does not explode. We therefore choose the signs

$$N(z) = \hat{N} \exp\left(\frac{-1 - i}{\sqrt{2}} \sqrt{\frac{|\omega|}{K}} z\right) \qquad (\omega > 0)$$

$$N(z) = \hat{N} \exp\left(\frac{-1 + i}{\sqrt{2}} \sqrt{\frac{|\omega|}{K}} z\right) \qquad (\omega < 0)$$
(15)

Because of the linearity of the heat equation, a multiple of a solution and the sum of two solutions in turn is a solution to the equation. With that we find that

$$T(t,z) = \int_0^\infty d\omega B_+(\omega) \exp\left(i\omega t + \frac{-1-i}{\sqrt{2}}\sqrt{\frac{\omega}{K}}z\right) + B_-(\omega) \exp\left(-i\omega t + \frac{-1+i}{\sqrt{2}}\sqrt{\frac{\omega}{K}}z\right)$$
(16)

one solution is what can be understood as a Fourier decomposition in time t. Using (16) we now look for the solution, which is the real harmonic boundary condition

$$T(t, z = 0) = \hat{T}\cos(\omega_o t) \tag{17}$$

Apparently this is the sum

$$T(t,z) = \hat{T} \exp\left(i\omega_o t + \frac{-1 - i}{\sqrt{2}} \sqrt{\frac{\omega_o}{K}} z\right) + \hat{T} \exp\left(-i\omega_o t + \frac{-1 + i}{\sqrt{2}} \sqrt{\frac{\omega_o}{K}} z\right)$$

$$= \hat{T} \exp\left(-\sqrt{\frac{\omega_o}{2K}} z\right) \cos\left(\omega_o t - \sqrt{\frac{\omega_o}{2K}} z\right)$$
(18)

The interpretation is that a harmonic change in temperature at the earth's surface in the depth z is perceived out of phase and attenuated. The time difference is

$$\Delta t(z) = \frac{z}{\sqrt{2\omega_o K}},\tag{19}$$

and the attenuation amounts to the factor

$$\exp\left(-\sqrt{\frac{\omega_o}{2K}}z\right). \tag{20}$$

Both are dependent on the excitation frequency  $\omega_0$ .

# 4 Classic billiards - statistical distributions

#### 4.1 Tasks

Simulate the movement of a given number of balls (10, 100, 1000) in a three-dimensional cuboid container. Apart from the balls there is nothing in the container, and gravitation should be neglected. This means that each ball moves between two impacts rectilinear uniform. Bumps take place between the balls and between walls. All collisions are said to be elastic, which means that the total kinetic energy is retained. Possible tasks are:

- Investigate whether for a given volume of the cube, a given number of particles and given total energy results in a pressure on the cube wall, which with the additional equation for ideal gases.
- Investigate after how many collisions the particles have forgotten their original speed. Make a histogram of the velocities of the particles and compare this with a Maxwell-Boltzmann distribution.
- Examine the number of particles in a partial volume of the cube and compare with statements of statistical thermodynamics about the fluctuations of the particle number in an open system<sup>2</sup>.
- Investigate the diffusion behavior of a subset of the particles. You decide a diffusion coefficient and compare with the theoretical expression.
- Investigate whether the totality of the particles according to the equation of state according to Van der Waals behave when the sum of the particle volumes is no longer negligible is significantly small compared to the volume in the cube.

# A Remarks on the numerical solving of (partial) differences, differential equations

#### A.1 Finite differences

Among many other numerical techniques, finite differences and finite elements are two Techniques for solving differential equations numerically.

- The "finite element" method is particularly popular in engineering, but not often found in physics. It is suitable for treatment of problems with complicated geometry in which bodies occur through an irregular grid of irregular tetrahedra can be represented. A big challenge in this context is the setting up of the grid. An example is the calculation of forces in the skull and the spine of a car driver in a rear-end collision (www.agu.ch). This method is not continued here.
- The "Finite Difference" method is based on (partial) derivatives through finite differences of function values at discrete points in the vicinity of the point at which the derivative is of interest. About this method, some remarks are made below.

The representation of the numerical values of a function of a continuous variable represents a computer is faced with a problem, because such a representation requires an infinite amount of memory. Therefore a program has to limit itself to making statements about the function in discreet places. This problem arises with every variable on which the function depends. For example, sometimes the discretization automatically creates a two-dimensional grid problems with a time and a space dimension. For the sake of simplicity, we assume that this lattice is equidistant in both dimensions.  $(x_{k+1}-x_k=\Delta x={\rm const}\ ,\,t_{n+1}-t_n=\Delta t={\rm const}\ )$ , where  $x_k$  and  $t_n$  are the discrete places and times. We use the notation

$$f_n^k := f(n \ \Delta t, k \ \Delta x). \tag{21}$$

for the function value at the point  $(n \Delta t, k \Delta x)$ .

In a differential equation there are derivatives like  $\partial f(t,x)/\partial x$ . It is the essence of the finite differences, such derivatives with suitable combinations of function values to describe. For this purpose we consider the Taylor approximation

$$f_{k+1}^n = f_k^n + \Delta x \frac{\partial f(t, x)}{\partial x} + \mathcal{O}(\Delta x^2)$$
 (22)

 $<sup>^2{\</sup>rm See}$  for example Bebie script: Statistical Thermodynamics II.

Obviously we can derive from this an expression for the first derivative with respect to x:

$$\left(\frac{\partial f(t,x)}{\partial x}\right)_{k}^{n} = \frac{f_{k+1}^{n} - f_{k}^{n}}{\Delta x} + \mathcal{O}(\Delta x) \tag{23}$$

The error of this approximation is of the order of magnitude of  $\Delta x$  and can therefore in principle can be made arbitrarily small. Contains a procedure expressions of the kind right page, it is called the first-order procedure in x. But let's go from the Taylor approximation

$$f_{k-1}^n = f_k^n - \Delta x \frac{\partial f(t, x)}{\partial x} + \mathcal{O}(\Delta x^2)$$
 (24)

we find an alternative expression for the first derivative

$$\left(\frac{\partial f(t,x)}{\partial x}\right)_{k}^{n} = \frac{f_{k}^{n} - f_{k-1}^{n}}{\Delta x} + O(\Delta x),\tag{25}$$

which is also of the first order. What both approaches have in common is that they rely on a two-point carry out the procedure (two neighboring points from the environment are used), and that they are first order. We now want to construct a second order expression for the derivative with respect to x. In addition, we should from the assumption  $af_{k-1}^n + bf_k^n + cf_{k+1}$  can be assumed. The constants a, b and c are initially unknown, the task is to determine this skillfully. We use again the Taylor approximations for  $f_{k-1}^n$  and  $f_{k+1}^n$ , but do not break until the fourth order and put in the above sum. After sorting according to derivatives, we get

$$af_{k-1}^{n} + bf_{k}^{n} + cf_{k+1}^{n} = (a+b+c)f_{k}^{n} + (-a+c)\Delta x \left(\frac{\partial f(t,x)}{\partial x}\right)_{k}^{n} + (a+c)\frac{\Delta x^{2}}{2} \left(\frac{\partial^{2} f(t,x)}{\partial x^{2}}\right)_{k}^{n} + (a-c)\frac{\Delta x^{3}}{6} \left(\frac{\partial^{3} f(t,x)}{\partial x^{3}}\right)_{k}^{n} + \mathcal{O}(\Delta x^{4})$$

$$(26)$$

The idea now is that the right side should represent the first derivative with respect to x. We choose a, b and c in such a way that the coefficients of as many other terms as possible vanish. How get the equations

$$a+b+c = 0$$

$$(-a+c)\Delta x = 1$$

$$a+c = 0$$
(27)

The representation follows immediately

$$\left(\frac{\partial f(t,x)}{\partial x}\right)_{k}^{n} = \frac{f^{n}k + 1 - f^{n}k - 1}{2\Delta x} + \mathcal{O}(\Delta x^{2})$$
(28)

The order of the error is now two, so it is a second order scheme. The same approach lists as the expression for the second derivative

$$\left(\frac{\partial^2 f(t,x)}{\partial x^2}\right)_k^n = \frac{f_{k+1}^n - 2f_k^n + f_{k-1}^n}{\Delta x^2} + \mathcal{O}(\Delta x^2).$$
(29)

Exercise: Derive this and explain why the error term is second and not first order in  $\Delta x$ . With an approach that takes more than three support points into account, one can in principle get involved establish a higher order scheme. At least two problems arise here. There, on the one hand, a large number of terms has to be evaluated, the calculation takes comparatively long. On the other hand, many support points mean that information from a larger area is incorporated into the determination of the derivative. Thereby the locality of the derivation gets lost what is especially near not nice flat features, especially with jumps have a negative effect.

# A.2 Application to the heat conduction equation

We consider the diffusion equation in one dimension

$$\frac{\partial f(t,x)}{\partial t} = D \frac{\partial^2 f(t,x)}{\partial x^2} \tag{30}$$

with Dirichlet boundary conditions f(t, x = 0) = b(t), where b(t) is a given function, for example b(t) = 0. With the methods given in Section A.1 we set the derivation according to time and place, whereby in both cases we use the expressions second order, and receive

$$\frac{f_k^{n+1} - f_k^{n-1}}{2\Delta t} = D \frac{f_{k-1}^n - f_k^n + f_{k+1}^n}{\Delta x^2}.$$
 (31)

As the stability analysis according to Neumann (see for example Gershenfeld (2000, p. 79)) shows, is however, this method is numerically unstable. Exercise: show this. The procedure becomes conditionally stable if we use a first-order scheme for the time derivative, select:

$$\frac{f_k^{n+1} - f_k^n}{\Delta t} = D \frac{f_{k-1}^n - f_k^n + f_{k+1}^n}{\Delta x^2}$$
 (32)

Carry out a stability analysis here too. The result is that

$$\Delta t \le \frac{(\Delta x)^2}{2D} \tag{33}$$

must be so that the stability is guaranteed. This criterion writes an upper bound for the time step  $\Delta t$  with a given spatial resolution  $\Delta x$ . The problem with this is that the computing time to be expended can be large. The time it takes for a signal to appear by diffusion by a distance L has spread, is approximately  $L^2/D$ . By limiting (33) it follows that the total number of time steps must be approximately  $L^2/(\Delta x)^2 \gg 1$ ). The problem can also be expressed differently: Should the spatial resolution be one factor 2 must be improved according to the restriction (33)  $\Delta t$  by the factor 4 can be reduced in size. That means that you have to calculate about 8 times more. Conclusion: that procedure works numerically, but it can be slow. One way out of this problem are implicit procedures (Gershenfeld, 2000, p. 82). In implicit procedures are procedures in which the function value at one point leads to anew time  $t + \Delta t$  not only given by the function values at a previous time but depend on function values from the environment at the new time. This dependency leads to matrix equations, which can be solved quite easily with a trick. With regard to stability, implicit methods are often superior to explicit ones, for example, this means that there is no restriction for the time step  $\Delta t$  for reasons of stability.

- 1. Chowdhury, D., Santen, L., A. Schadschneider, Simulation of Vehicular Traffic: A.Statistical Physics Perspective, Computing in Science and Engineering, 2, 80-87, 2000
- 2. Gershenfeld, N., The Nature of Mathematical Modeling, Cambridge University Press, Cambridge, UK, 2000
- 3. Kühne, R., Traffic flow on trunk roads, driving a car as an example of nonlinear onesDynamics, phys. Bl. , 47, 201-204, 1991
- 4. Schreckenberger, M., A. Schadschneider, K. Nagel, simulating cellular automataRoad traffic, phys. Bl. , 52, 460-462, 1996