

Convection-diffusion simulation in two different dimensions

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This paper deals with the principle of groundwater pollution. The basic equation for pollution distribution is the diffusion equation. In the natural but also economical science different kinds of this equation are used. This work focuses on the convection-diffusion equation. Using this equation the diffusive behavior of the pollution influenced by a velocity field is described. Several approaches, ranging from analytical solutions to some chaotic particle movement approaches, are used for realization in one- and two-dimensional domains.

1 Introduction

In chemistry as well as in biology the reaction-diffusion equation plays a very important role. This equation can be used to recreate pattern formations of a fish' skin or cat's fur. There are also many physical applications of diffusion, e.g. the heat equation. However, diffusion is also used to foresee the behavior of buyers of stocks in the financial market. In the following the convection-diffusion equation is used.

$$\frac{\partial c}{\partial t} = D \cdot \nabla^2 c - v \cdot \nabla c \quad (1)$$

Equation (1) describes diffusive distribution influenced by a velocity field. The used velocity field is constant and only nonzero along x -direction. The groundwater pollution is a vivid application of (1).



Figure 1: A schematic illustration of the described area.

Instead of using a difficult realistic geometry of a surrounding a two-dimensional rectangle is considered.

This rectangle is embedded in a Cartesian coordinate system. In the origin a source of pollution is placed as shown in figure 1. There are two different types of source. On the one hand a constantly releasing pollution source can be used. On the other hand the pollution distribution of an instantaneous releasing source can be considered. In the following the second kind of source is used for various simulation approaches in one and two dimensions.

2 Analytical Solution

Usually it is not easy or even possible to find an analytical solution. Due to the used initial and boundary conditions an analytical solution can be given. Both solutions, one- and two-dimensional, are used to validate the different methods.

2.1 One-dimensional

The regarded equation and its condition are given as follows

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - v \frac{\partial c}{\partial x} \quad \text{with} \quad c(x,0) = \delta(x) \quad (2)$$
$$\lim_{x \rightarrow \pm\infty} c(x,t) = 0.$$

Using different substitutions [1] the equation (2) can be written as

$$\begin{aligned} \tau &= Dt, & b &= \frac{v}{D} \\ y &= x - b\tau, & y_0 &= b\tau_0 \\ \frac{\partial c(y, \tau)}{\partial \tau} &= \frac{\partial^2 c(y, \tau)}{\partial y^2}. \end{aligned} \quad (3)$$

After multiplying equation (3) by $e^{-p\tau}$ and integrating it with respect to τ one obtains an ordinary differential equation which can be easily solved. Using the inverse Laplace-transformation and the substitutions backwards we obtain the solution of the one-dimensional problem.

$$c(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-vt)^2}{4Dt}} \quad (4)$$

2.2 Two-dimensional

In order to solve the two-dimensional equation

$$\begin{aligned} \frac{\partial c}{\partial t} &= D \cdot \frac{\partial^2 c}{\partial x^2} + D \cdot \frac{\partial^2 c}{\partial y^2} - v \cdot \frac{\partial c}{\partial x} \quad \text{with} \\ c(x_0, y_0, 0) &= \delta(x)\delta(y) \\ \lim_{x, y \rightarrow \infty} c(x, y, t) &= 0 \\ \lim_{x, y \rightarrow -\infty} c(x, y, t) &= 0 \end{aligned} \quad (5)$$

a solution of the following form is assumed. [2]

$$c(x, y, t) = g_1(x, x_0, t)g_2(y, y_0, t) \quad (6)$$

The functions g_1 and g_2 are solutions of the one-dimensional convection-diffusion equation with constant coefficients. Therefore g_1 and g_2 can be taken from the one-dimensional analytical solution (4).

$$\begin{aligned} g_1(x, x_0, t) &= \frac{A_1}{2\sqrt{D\pi t}} \exp\left(\frac{-(x-x_0-vt)^2}{4Dt}\right) \\ g_2(y, y_0, t) &= \frac{A_2}{2\sqrt{D\pi t}} \exp\left(\frac{-(y-y_0)^2}{4Dt}\right) \end{aligned} \quad (7)$$

The source is located at the origin therefore the values $x_0 = 0$ and $y_0 = 0$ can be inserted. Additionally the integral over the whole domain has to be 1.

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c(x, y, t) dx dy = \\ &= \int_{-\infty}^{\infty} g_1(x, 0, t) dx \int_{-\infty}^{\infty} g_2(y, 0, t) dy = A_1 A_2 \end{aligned} \quad (8)$$

This integration result leads to the analytical solution in two dimensions.

$$c(x, y, t) = \frac{1}{4D\pi t} \exp\left(\frac{-(x-vt)^2 - y^2}{4Dt}\right) \quad (9)$$

3 Numerical Approximation

This section introduces two types of numerical approximations. On the one hand there is the finite difference method (FDM). In this approximation the derivative of the differential equation is approached by taking the difference quotient of the neighboring grid points. The method is easy to use but slightly weak concerning the accuracy. The second method is the finite element method (FEM) and is based on formulating variations of the differential equation. FEM determines approximated solutions consisting of piecewise defined polynomials on a fine resolution of the domain. The advantage of FEM is the suitability for any geometry.

3.1 Finite Difference Method

The finite difference method is implemented for the one- and two-dimensional case.

3.1.1 One-dimensional

Using finite differences to approximate the first and second derivatives the partial differential equation (1) transforms into an ordinary differential equation.

$$\frac{dc}{dt} = D \cdot \frac{c_{i+1} - 2c_i + c_{i-1}}{x^2} - v \cdot \frac{c_i - c_{i-1}}{dx} \quad (10)$$

The time derivative can be replaced as follows

$$\frac{dc}{dt} = \frac{c^{k+1} - c^k}{\Delta t}. \quad (11)$$

Using (11) equation (10) can also be written as a matrix product

$$\frac{c^{k+1} - c^k}{\Delta t} = S \cdot c^k = S \cdot \begin{pmatrix} c_1 \\ \vdots \\ c_n \end{pmatrix} \quad (12)$$

with

$$S := \begin{pmatrix} -\frac{D}{h^2} + \frac{v}{h} & \frac{2D}{h^2} - \frac{v}{h} & 0 & \dots & 0 \\ \frac{D}{h^2} + \frac{v}{h} & \frac{2D}{h^2} - \frac{v}{h} & \frac{D}{h^2} & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \frac{D}{h^2} + \frac{v}{h} & \frac{2D}{h^2} - \frac{v}{h} & \frac{D}{h^2} \\ 0 & \dots & 0 & -\frac{D}{h^2} + \frac{v}{h} & \frac{D}{h^2} - \frac{v}{h} \end{pmatrix}$$

whereas c^k is the current concentration of pollution and c^{k+1} the concentration in the next time step. In order to determine c^{k+1} using the Explicit Euler equation (12) is rearranged.

$$c^{k+1} = (\Delta t S + I) c^k \quad (13)$$

It is well known that the Explicit Euler can be unstable using the wrong step size relation. Notation (12) can be also used to find the Implicit Euler formulation. The current concentration on the right hand side in equation (12) is replaced by the concentration of the future time step in order to obtain the implicit formulation.

$$c^{k+1} = (I - \Delta t S)^{-1} c^k \quad (14)$$

3.1.2 Two-dimensional

Regarding the problem formulation in two dimensions the finite difference method looks a little bit different. Due to the fact that an equidistant grid, $dx = dy$ is used the approximation can be given as follows

$$\frac{dc}{dt} = D \cdot \frac{c_{x+1,y} + c_{x-1,y} - 4c_{x,y} + c_{x,y+1} + c_{x,y-1}}{dx^2} - v \frac{c_{x,y} - c_{x-1,y}}{dx}. \quad (15)$$

In contrary to the two-dimensional case the matrix notation is not as easy as in one dimension.

$$c_{x,y}(t + \Delta t) = c_{x,y}(t) + h \cdot \frac{dc}{dt} \quad (16)$$

Therefore only the Explicit Euler method is implemented as shown in (15).

3.2 Finite Element Method

The finite element method was only realized for the convection-diffusion equation in one dimension.

$$\begin{aligned} \frac{\partial c}{\partial t} - D \frac{\partial^2 c}{\partial x^2} + v \frac{\partial c}{\partial x} &= 0 & \text{in } \Omega \\ c &= 0 & \text{on } \partial\Omega \end{aligned} \quad (17)$$

First of all the weak solution of (17) is formalized using a test function of the according Sobolev space $\phi \in H_0^1$.

$$\int_{\Omega} \frac{\partial c}{\partial t} \phi d\Omega + \int_{\Omega} (D \nabla c \nabla \phi + v \nabla c \phi) d\Omega = 0 \quad (18)$$

The formulation of the Galerkin approximation is necessary to formulate the solution equation of the finite element method.

$$c^n(x) = \sum_{j=1}^n c_j \varphi_j(x) + c_0(x) \quad (19)$$

The unknown variables c_j in equation (19) have to be determined. Using linear basis functions called 'hat-functions' for ϕ a linear system of n equations with

n unknowns, called the Galerkin formulation, results. [3]

$$\begin{aligned} \sum_{j=1}^{n_e} \frac{\partial c_j}{\partial t} \int_{\Omega^{e_k}} \varphi_j \varphi_i d\Omega \\ + \sum_{j=1}^{n_e} c_j \int_{\Omega^{e_k}} (D \nabla \varphi_j \nabla \varphi_i + \nabla \varphi_j \varphi_i) d\Omega = 0 \end{aligned} \quad (20)$$

In equation (20) n_e is the number of elements in every finite element and Ω^{e_k} is the domain of element e_k . Equation (20) can also be written in a short form.

$$\begin{aligned} \dot{c} \cdot M + c \cdot S = 0 \quad \text{with} \\ m_{ij} = \int_{\Omega^{e_k}} \varphi_i \varphi_j d\Omega \\ s_{ij} = \int_{\Omega^{e_k}} (D \nabla \varphi_i \nabla \varphi_j + \nabla \varphi_i \varphi_j) d\Omega \end{aligned} \quad (21)$$

The matrices of (21) are called mass matrix M and stiffness matrix S . Considering the mentioned 'hat-functions' it is clear, that only a few of the possible integrals are not equal zero. Those basis functions which correspond to the corner points of the element will lead to non trivial results. Because the element i is connected to $i-1$ and $i+1$ the profile of the matrices is a band matrix with width three.

$$M \frac{c^{k+1} - c^k}{\Delta t} + \theta S c^{k+1} + (1 - \theta) S c^k = 0, \quad 0 \leq \theta \leq 1 \quad (22)$$

Equation (22) is called θ -method and will be used to present implicit and explicit methods for solving (21). The most common values for θ are:

- $\theta = 0$, Explicit Euler
- $\theta = 1$, Implicit Euler
- $\theta = \frac{1}{2}$, Implicit Heun

Using this method the Explicit and Implicit Euler algorithm can be given.

$$c^{k+1} = M^{-1} (M - \Delta t S) c^k \quad (23)$$

$$c^{k+1} = (M + \Delta t S)^{-1} M c^k \quad (24)$$

4 Random Walk

An alternative method for simulating transport is the so-called random walk. This approach is contrary to the numerical solutions. The focus changes from a macroscopic view to the simulation of microscopic behavior of diffusion by analyzing movements of single particles.

4.1 Intuitive Approach

The intuitive approach describes a model which uses no grid or collision rules. It is implemented again for both dimensions.

4.1.1 One-dimensional

At the beginning $t = 0$ all the particles are placed in the origin presenting the source of pollution. The pollution injection happens only at $t = 0$. The simulation focuses on the convection and diffusion behavior of these initial particles. In this approach the movement of particles is described by:

$$\begin{aligned} p_{new} &= p_{old} + r + v \cdot \Delta t \\ r &= X \cdot \Delta x \end{aligned} \quad (25)$$

The particle motion in (25) consists of three parts. In order to get the new position p_{new} at time $t + \Delta t$ these three components are summed up. The variable p_{old} stands for the position at time t . The velocity field v is multiplied by the step size. The variable r describes the diffusive movement of a particle for one time step and is added to the former particle position p_{old} . The second equation in (25) defines the movement r in particular. It consists of the step size in space Δx and a normally distributed random variable X with mean zero and unit variance. In every time step the new position of every particle is calculated with equation (25). The simulation ends when the chosen simulation time t_{end} is reached.

4.1.2 Two-dimensional

For expansion in a two-dimensional domain the movement has to be defined in a different way. There is no

initial velocity but there is an initial direction of every particle d_0 . The diffusive transport is realized by using a normally distributed random variable X and a uniformly distributed random number U . X is used to generate a random length and U chooses a coincidental direction.

$$r = X \cdot \Delta x \quad \alpha = U \cdot 2\pi$$

$$d_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad d_{n+1} = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \cdot d_n \quad (26)$$

In (26) r stands for the distance the particle moves in a certain time step. The influence of this parameter is similar to the diffusion coefficient. X is the mentioned normally distributed random variable and Δx describes the step size in space. The second equation of (26) sets the direction for the particle's next move. The initial direction d_0 is only necessary for the recursive definition. During simulation the direction of the last movement is used to calculate the next one. The convection is realized by a shift in flow direction along x . The final formulation of the random walk movement can be given as follows

$$p_{new} = p_{old} + d \cdot r + vdt. \quad (27)$$

4.2 Gaussian Approach

This approach shows the connection between a random walk approach and the analytical solution.

4.2.1 One-dimensional

The analytical solution of the convection-diffusion equation (2) is used to define the particle movement. Considering the probability density function of a normal or Gaussian distribution

$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad (28)$$

the formal equivalence to the analytical solution (4) is obvious. The parameters used in (28) stand for the mean value μ and the standard deviation σ which characterize the position and the width of the Gaussian

bell curve in a unique way. Therefore the according parameters in (4) can be read out. [4]

$$\mu = v \cdot t$$

$$\sigma^2 = 2 \cdot Dt \quad (29)$$

Due to the properties and meaning of the parameters in (29) the height and width of the concentration peak depending on time is given. The corresponding particle movement using (29) can be formulated as follows

$$p_{new} = p_{old} + v\Delta t + \sqrt{2 \cdot D\Delta t}X. \quad (30)$$

The variable X stands for a normally distributed random number with mean zero and unit variance as in the intuitive approach. X is newly generated in every step for each particle. Identifiable by the velocity v the second term stands for the convective motion. This term is equal to the term of the intuitive approach. The radical term describes the diffusive motion and is based on the standard derivation.

4.2.2 Two-dimensional

In order to enlarge this approach in two dimensions the movement along y -direction has to be added. For an expansion in a two-dimensional domain the y -component of the movement has to be defined. Due to the fact that there is no flux the new particle position can be calculated using

$$p_x^{new} = p_x^{old} + v\Delta t + \sqrt{2 \cdot D\Delta t}X_x$$

$$p_y^{new} = p_y^{old} + \sqrt{2 \cdot D\Delta t}X_y. \quad (31)$$

The variables X_x and X_y stand for independent normally distributed random numbers which are newly generated in every step for each particle. The term $v\Delta t$ describes the convective transport. Due to the fact that the diffusion coefficient is equal for the x - and y -direction the diffusive movement $\sqrt{2 \cdot D\Delta t}$ in the random walk definition (31) is the same.

5 Results

In the following section the analytical solutions in both dimensions are compared to the various approaches. The different concentration errors are discussed. In general the parameter setting is: diffusion coefficient $D = 0.02$ and velocity $v = 0.02$. The step sizes Δt and Δx are variable. The regarded simulation time varies between $t_{end} = 250$ and $t_{end} = 500$.

5.1 Analytical vs. Numerical

First of all the numerical solutions are considered.

5.1.1 FDM 1D

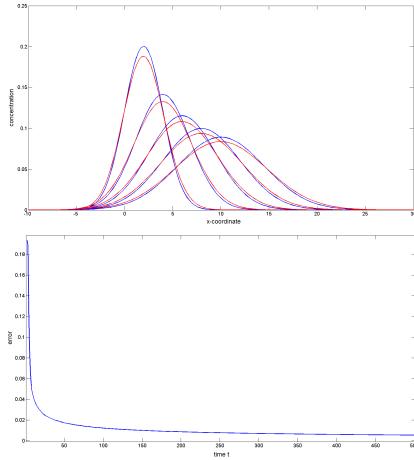


Figure 2: Comparison of the analytical solution and FDM using matrix notation.

In the upper plot in figure 2 the red curve is the analytical solution and the blue line sketches the numerical approximation using the Implicit Euler algorithm. In the lower plot the difference of both solutions is shown.

The results in table 1 show the instability of the Explicit Euler method. The Implicit Euler algorithm is not only ultra-stable but also faster and more exact than the Explicit Euler. The approximation using finite differences is well-fitting.

Δt	Δx	Explicit Euler		Implicit Euler	
		$\ \cdot\ _\infty$	$\ \cdot\ _1$	$\ \cdot\ _\infty$	$\ \cdot\ _1$
1	1	0.016	$4.231E^{-4}$	0.016	$4.753E^{-4}$
1	$\frac{1}{2}$	0.009	$1.404E^{-4}$	0.010	$1.600E^{-4}$
$\frac{1}{2}$	$\frac{1}{4}$	0.005	$0.831E^{-5}$	0.005	$7.323E^{-5}$
$\frac{1}{2}$	$\frac{1}{16}$	NaN	NaN	0.002	$3.531E^{-5}$

Table 1: Error values of FEM using Explicit and Implicit Euler.

5.1.2 FDM 2D

The results regarding the two-dimensional implementation show a similar behavior.

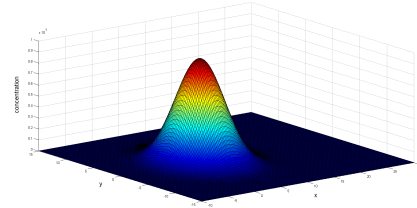


Figure 3: The analytical and numerical solution is shown.

In figure 3 the surface plot shows the concentration of the numerical result. In the following the error values are studied in detail.

Δt	Δx	explicit Euler	
		$\ \cdot\ _\infty$	$\ \cdot\ _1$
1	1	0.0027	$1.5624E^{-4}$
$\frac{1}{2}$	$\frac{1}{4}$	$9.1479E^{-4}$	$1.4640E^{-5}$
1	$\frac{1}{2}$	0.0017	$3.7791E^{-5}$
$\frac{1}{4}$	$\frac{1}{8}$	$.E^{119}$	$.E^{120}$
$\frac{1}{2}$	$\frac{1}{2}$	0.0016	$3.8172E^{-4}$
$\frac{1}{8}$	$\frac{1}{8}$	$4.7570E^{-4}$	$8.5291E^{-6}$
1	$\frac{1}{4}$	$.E^{32}$	$.E^{33}$

Table 2: The error values for FDM using Explicit Euler are shown.

Also in the two-dimensional case the Explicit Euler works not for all parameter choices. The error values are again quite good. The finite difference method of the two-dimensional domain approximates

the convection-diffusion equation in an appropriate way.

5.1.3 FEM 1D

The accuracy of the finite element method is better than of the finite difference method.

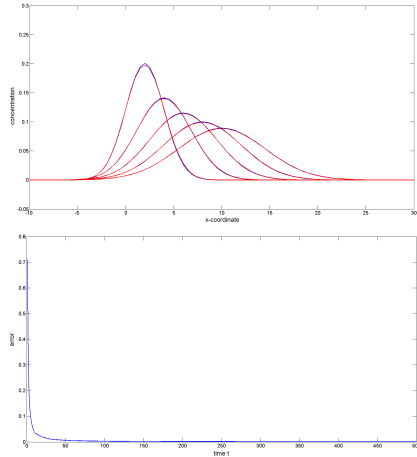


Figure 4: The error for the Implicit Euler algorithm of the FEM is shown.

In figure 4 above the upper plot shows the analytical solution as well as the finite element method using Implicit Euler. It is hard to distinguish the different curves.

Δt	Δx	Explicit Euler		Implicit Euler	
		$\ \cdot\ _\infty$	$\ \cdot\ _1$	$\ \cdot\ _\infty$	$\ \cdot\ _1$
1	1	$7.18E^{-4}$	$3.16E^{-5}$	$9.95E^{-4}$	$3.03E^{-5}$
1	$\frac{1}{2}$	$6.23E^{-4}$	$8.60E^{-5}$	$6.09E^{-4}$	$8.54E^{-5}$
$\frac{1}{2}$	$\frac{1}{4}$	$3.13E^{-4}$	$1.02E^{-4}$	$2.74E^{-4}$	$1.01E^{-4}$
$\frac{1}{2}$	$\frac{1}{8}$	NaN	NaN	$2.49E^{-4}$	$1.05E^{-4}$

Table 3: Depending on the used FEM the error values are shown.

The instability of the Implicit Euler is shown in the last row of table 3. In general the error results are smaller compared to the results of the finite difference method in one dimension. The finite element method approximates the convection-diffusion equation better than the finite difference method.

5.2 Analytical vs. Stochastic

The accuracy of the random walk approaches is discussed in the following paragraph.

5.2.1 One-dimensional

The two random walk implementations are compared to the analytical solution.

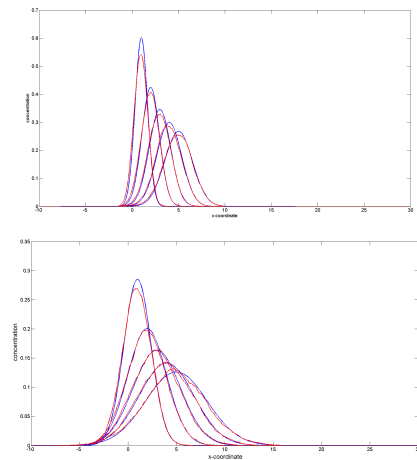


Figure 5: Comparison of intuitive and stochastic based random walk are shown.

The two graphics in figure 5 show both random walk approaches colored in red and the analytical solution in blue. In the upper plot the intuitive implementation is shown. The lower plot sketches the Gaussian-based version of random walk. In the numerical comparisons the simulation time is $t_{end} = 500s$. Due to long execution times for the particle movement this parameter is reduced to $t_{end} = 250s$. The diffusion coefficient is usually set to $D = 0.02$ but modifies if the intuitive approach is used.

The table 4 shows all the error results of the parameter study comparing the analytical solution and both random walk approaches. Adapting the diffusion coefficient both approaches fues into one single random walk implementation. The diffusion coefficient for the Gaussian-based algorithm is set to $D = 0.02$. Using the intuitive approach the diffusion coefficient of the analytical solution changes to D^* to enables comparability. Due to the dependency on Δx and Δt the intuitive random walk cannot reach its performance. On

Δt	Δx	D^*	intuitive RW		Gaussian RW	
			$\ \cdot\ _\infty$	$\ \cdot\ _1$	$\ \cdot\ _\infty$	$\ \cdot\ _1$
1	$\frac{1}{5}$	0.01	0.007	$8.948E^{-7}$	0.012	$8.948E^{-7}$
1	$\frac{1}{10}$	0.005	0.014	$4.441E^{-16}$	0.008	$9.707E^{-7}$
$\frac{1}{2}$	$\frac{1}{5}$	0.04	0.006	$3.342E^{-5}$	0.007	$8.948E^{-7}$
$\frac{1}{2}$	$\frac{1}{10}$	0.01	0.009	$8.419E^{-12}$	0.010	$9.707E^{-7}$
$\frac{1}{2}$	$\frac{1}{15}$	0.0045	0.016	$8.882E^{-16}$	0.009	$9.969E^{-7}$
1	$\frac{1}{5}$	0.01	0.010	$0.948E^{-7}$	0.007	$8.948E^{-7}$
1	$\frac{1}{10}$	0.005	0.015	$6.661E^{-16}$	0.005	$9.707E^{-7}$

Table 4: Comparison of the random walk approaches and the analytical solution.

contrary a parameter study would be necessary to find the perfect variable value for all step size combinations to perform this algorithm. Therefore, regarding simulation of the convection-diffusion equation, the implementation of the Gaussian-based random walk fits better. In the last two rows the used particle number is raised from 6000 to 8000.

5.2.2 Two-dimensional

In order to compare the analytical solution to a random walk approach the results have to be adapted. In the random walk the output describes the smoothed amount of particles in every cell. Due to the initial Dirac-function the integral at the beginning has value one. The area of the random walk domain is discretized. Therefore the output has to be divided not only by the number of particles but also by the area of the cells used for the flattening.

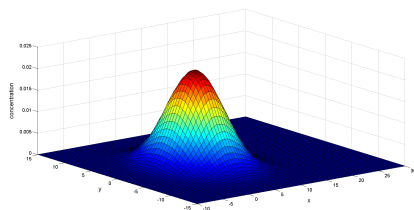


Figure 6: Analytical and Gaussian solution are shown.

Figure 6 shows the concentration results of the random walk approach. The difference between these two implementations cannot be read out exactly. Therefore a closer look to the simulation data itself is given.

Table 5 shows the approximation results. The parameter r describes the used radius for the flattening. If the

Δt	Δx	r	N	Gaussian RW	
				$\ \cdot\ _\infty$	$\ \cdot\ _1$
1	1	3	4000	$3.395E^{-3}$	$6.349E^{-4}$
1	$\frac{1}{2}$	8	4000	$5.033E^{-3}$	$3.737E^{-5}$
$\frac{1}{2}$	$\frac{1}{2}$	15	4000	$1.063E^{-2}$	$1.071E^{-3}$
$\frac{1}{2}$	$\frac{1}{4}$	15	4000	$4.526E^{-3}$	$1.005E^{-4}$
$\frac{1}{2}$	$\frac{1}{8}$	20	4000	$2.801E^{-3}$	$2.206E^{-3}$
1	$\frac{1}{4}$	20	8000	$6.764E^{-3}$	$3.338E^{-5}$
$\frac{1}{2}$	$\frac{1}{4}$	20	8000	$6.825E^{-3}$	$1.826E^{-4}$

Table 5: Error values for the Gaussian approach are shown.

spatial step size is decreasing a greater radius r can be used. If r is chosen too big compared to Δx the result loses the shape of a bell curve. Compared to the results of the numerical simulation the random walk approach leads to greater error values.

6 Conclusion

In general the finite element method approximates the convection-diffusion equation the best. Of course the very best solution is the analytical one. In spite of it all random walk approaches are quite good approximations of the convection-diffusion equation.

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