

New Analytical Results and Numerical Schemes for Irregular Diffusion Processes

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Abstract

We examine the transient diffusion equation with time- and space-dependent diffusion coefficients in 1D. Such transport equations can be easily derived from the Fokker-Planck equation and are essential to understand the diffusion mechanisms in general, e.g. in carbon nanotubes. With the help of the classical self-similar Ansatz we give new, nontrivial analytical solutions. Then we reproduce these by 16 explicit numerical time integration methods, 11 of which are recent and unconditionally stable. The results show that some of the algorithms, e.g. the leapfrog-hopscotch method, are very efficient and can outperform the standard FTCS method.

Keywords

Diffusion equation; analytical solutions; numerical methods; time-dependent diffusion coefficient; space-dependent diffusion coefficient

1. Introduction

Regular diffusion or regular heat conduction is an important transport process which can occur in solids. It is described with a single linear partial differential equation (PDE) of space and time. Diffusion means particle transport and heat conduction means energy transport. Generally, diffusion processes can be studied in different coordinate systems with different dimensions, here we consider only one Cartesian coordinate, therefore the simplest diffusion PDE reads

$$\frac{\partial u(x,t)}{\partial t} = D \frac{\partial^2 u(x,t)}{\partial x^2} \quad (1)$$

where $x, t \in \mathbb{R}$, $u = u(x, t)$ is the distribution of the particle concentration (temperature in case of heat conduction) in space and time and D is the constant diffusion coefficient.

Plenty of analytical solutions exist for Eq. (1). On the other hand, simple equations such as (1) are often considered to construct and test new numerical algorithms by mathematicians. However, in real problems, the properties of the materials such as the diffusivity are rarely constant, but depend on time [1] or space. The general space-dependent diffusion equation, which is also called the Fick-Jacobs equation [2] (p. 68) are usually derived from the Fokker-Planck equation as it was shown by Reguera and Rubi [3] or by Zwanzig [4]. Such equations are used to describe the single-particle diffusion processes in systems with structural inhomogeneities like narrow ribbon channels [5]. These kinds of systems emerge when molecules move through carbon nanotubes [6], the membrane of cells [7] or systems of channels e.g. in zeolites [8].

To introduce and investigate irregular diffusion phenomena, we define the PDE (1) with non-constant diffusion coefficients. More concretely, the diffusion coefficient will have the simple power law time or space dependence: $D(t) = \hat{D}t^n$ or $D(x) = \bar{D}x^m$. In these two cases, the diffusion equation have the form of

$$\frac{\partial u(x, t)}{\partial t} = \hat{D} t^n \frac{\partial^2 u(x, t)}{\partial x^2}, \quad (2)$$

and

$$\frac{\partial u(x, t)}{\partial t} = \bar{D} \frac{\partial}{\partial x} \left(x^m \frac{\partial u(x, t)}{\partial x} \right) = \bar{D} \left(mx^{m-1} \frac{\partial u(x, t)}{\partial x} + x^m \frac{\partial^2 u(x, t)}{\partial x^2} \right), \quad (3)$$

respectively. To avoid confusion, we use the \hat{D} and \bar{D} notations for the constant ‘‘generalized diffusion coefficient’’ in the time and space dependent cases, thus they have the dimension of $t^{-n}D$ and $x^{-m}D$, respectively.

In two of our last studies [9], [10] we investigated the regular diffusion equation of Eq. (1) with the above-given self-similar, traveling wave, traveling profile or with some generalized self-similar Ansätze. We derived some new analytical solutions for the regular diffusion equation which go far beyond the well-known Gaussian (and error-type) solutions and can be expressed with the multiplication of Gaussian and Whittaker or Kummer's functions including different parameters. The presented and analysed refined functions describe irregular solutions, which have a different rate of decay than the Gaussian fundamental solution. Additionally, we evaluated solutions which have some oscillatory behaviour and a quick decay at large temporal and spatial coordinates. Some other solutions have physical relevance and describe power-law decay processes at infinite time and space coordinates. In the present paper, we investigate the diffusion equation which has spatial dependent diffusion coefficients, we solve it with the classical self-similar Ansatz and analyse the possible solutions, which contain the Whittaker functions. We will show that due to the additional exponential factor in the Whittaker functions have a much quicker decay than the Kummer functions (see Eq. (4)). Such kinds of solutions for diffusion processes are still unknown in the scientific literature till now.

There is a detailed study by Bluman and Cole [11] describing several analytical solutions to the diffusion equation - very similar to the error functions - but our results are novel and different from those of [11]. Straightforward generalizations of diffusion equations are the reaction (or) advection-diffusion equations. Such systems may have spatially dependent velocity or diffusion coefficients as well. Zoppou and Knight managed to derive analytical solutions for such a system [12]. However, their solutions are different from ours because they used a Gaussian-type Ansatz and not our general self-similar type. To find an analogy, we should mention that for the incompressible multi-dimensional Navier-Stokes equation the analytic results [13] derived from the self-similar Ansatz are the Kummer functions [14]. For the compressible case, however, the Whittaker function was obtained [15]. In this sense, we

have to emphasize that for processes where the diffusion coefficient has spatial dependence, the resulting functions to a great extent are different from the time dependent case (for this latter case, consult [16]).

Most numerical methods to solve the diffusion or heat conduction equation are either the member of the family of finite difference schemes (FDM) [17], [18] or that of finite element methods (FEM) [19], [20], or a mixture of these [21]. The best known FDMs are the explicit FTCS (forward time, central space), which uses the explicit Euler time discretization, and the implicit (Euler) and the Crank-Nicolson method. Implicit methods have much superior stability properties, thus they are typically used to solve this and similar equations [22]–[31]. Their disadvantage is that they require the solution of a system of algebraic equations at each time step, whose parallelization is not obvious. Explicit methods avoid this problem, but most of them are unstable when the time step size is larger than the so-called CFL (Courant–Friedrichs–Lewy) limit. This limit can be very low for non-uniform systems, e.g. in the case of Eq. (2) and (3), which will be demonstrated in Section 4 of the current paper.

That is why we agree with those scholars who think that explicit and unconditionally stable algorithms are worth to study [32]–[39]. In the recent past we constructed new specimens of this family, theoretically studied and tested them using simple analytical solutions, as well as numerical reference solutions [16], [40]–[47]. We found that these new methods are able to give fairly accurate results much faster than other methods or the widely used MATLAB ‘ode’ solvers. In this paper, we use the constructed nontrivial analytical solutions to examine how the methods perform and which one can be proposed under different circumstances.

2. The analytical solutions

We solve PDE (1), (2) and (3) using the well-known reduction technique. First a new variable $\eta = \frac{x}{t^b}$ is defined, which is a combination of the space and time variable. The solution $u(x, t)$ is then searched with the self-similar Ansatz, which has the form

$$u(x, t) = t^{-a} f(\eta) = t^{-a} f\left(x/t^b\right), \quad (4)$$

where a and b are arbitrary real constants (noted by α and β in our previous papers) and f is the shape function with one single variable η . The first and second derivatives with respect to η are denoted by f' and f'' . It is assumed that they exist and continuous.

2.1. The case of constant diffusion coefficient

If one substitutes the first and second derivative of the Ansatz (4) into the original Eq. (1) one obtains the following ordinary differential equation (ODE) for $f(\eta)$:

$$-af - \frac{1}{2}\eta f' = Df''.$$

However, this transformation is valid only if the following conditions are fulfilled: a is an arbitrary real number, $b = 1/2$. Now the software Maple12 gives the solution of this ODE:

$$f(\eta) = \eta e^{-\frac{\eta^2}{4D}} \left(c_1 M \left[1-a, \frac{3}{2}, \frac{\eta^2}{4} \right] + c_2 U \left[1-a, \frac{3}{2}, \frac{\eta^2}{4D} \right] \right)$$

where M and U are the Kummer M and U functions, respectively. For negative integer values of a , the solution can be written in another form:

$$f(\eta) = e^{-\frac{\eta^2}{4D}} \left(c_3 H_{2a-1} \left[\frac{\eta}{2\sqrt{D}} \right] + c_4 \cdot {}_1F_1 \left[\frac{1-2a}{2}, \frac{1}{2}; \frac{\eta^2}{4D} \right] \right),$$

where H is the Hermite polynomial, F is the hypergeometric function.

For $a = 4$ the solution can be simplified as follows:

$$u(x, t) = \frac{x}{t^{9/2}} \left(1 - \frac{x^2}{2Dt} + \frac{x^4}{20D^2t^2} - \frac{x^6}{840D^3t^3} \right) e^{-\frac{x^2}{4Dt}} \quad (5)$$

Fig. 1 shows the time development of the concentration function (5).

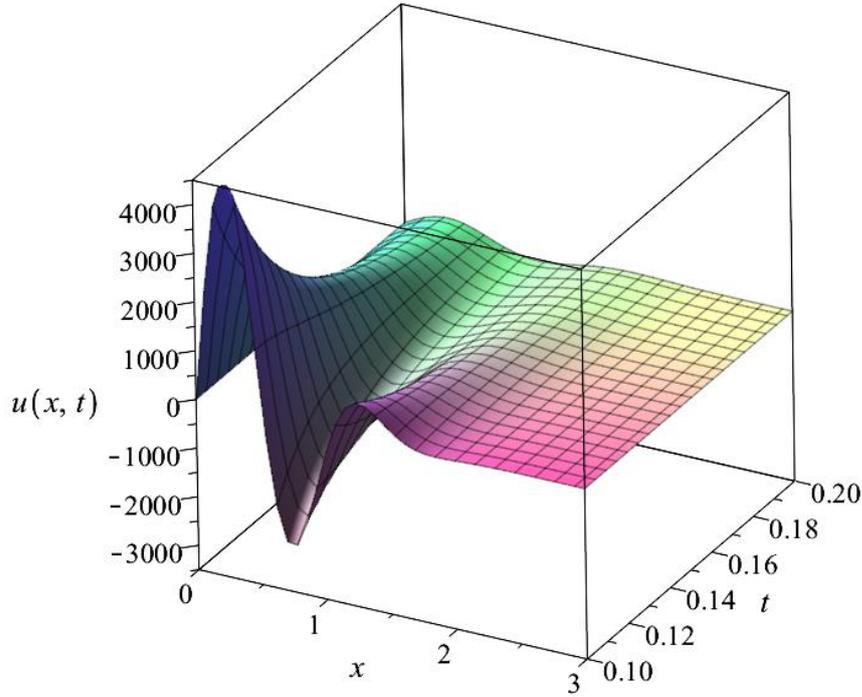


Fig. 1: The solution (5) of Eq. (1) in the case of constant diffusion coefficient for $D = 1$, $t \in [0.1, 0.2]$, $x \in [0, 3]$.

2.2. The case of time-dependent diffusion coefficient

Substituting the Ansatz (4) into PDE (2) yields the following ordinary differential equation (ODE) for $f(\eta)$:

$$-af - \frac{z}{2}\eta f' = \hat{D}f'',$$

if the following conditions are fulfilled: a is an arbitrary real number, $b = z/2$, where $z = n + 1$. The solution of this ODE:

$$f(\eta) = \eta e^{-\frac{z}{4\hat{D}}\eta^2} \left(c_1 M \left[\frac{z-a}{z}, \frac{3}{2}, \frac{z\eta^2}{4\hat{D}} \right] + c_2 U \left[\frac{z-a}{z}, \frac{3}{2}, \frac{z\eta^2}{4\hat{D}} \right] \right).$$

An example for the time development of the concentration function u for a given parameter set is presented in Fig. 2.

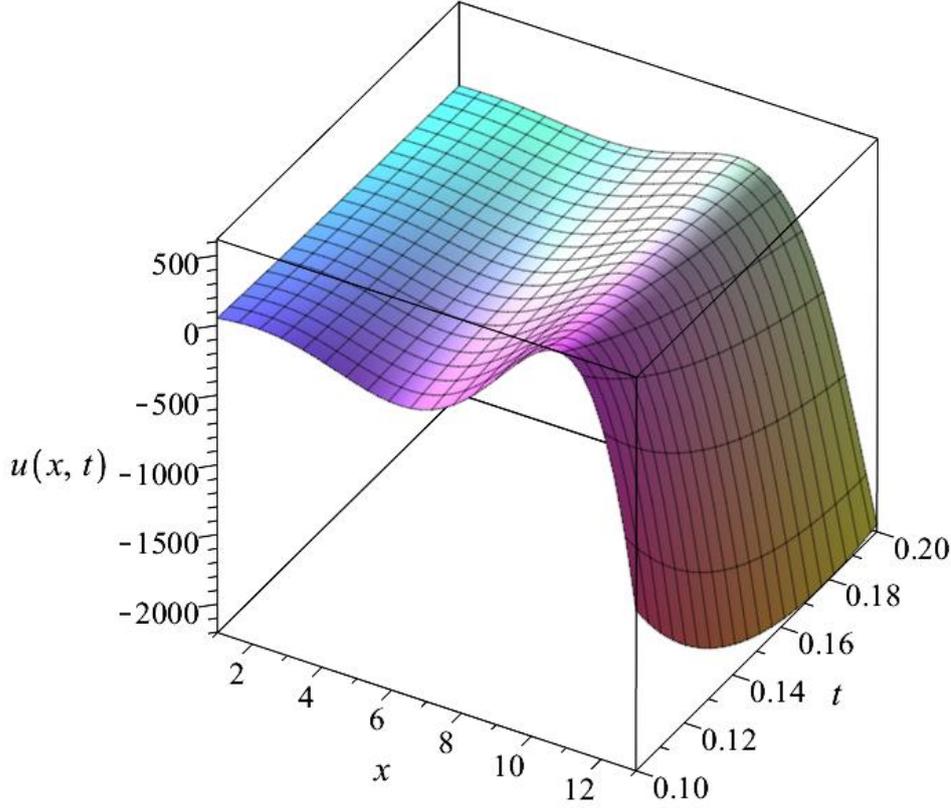


Fig. 2: The exploding solution of Eq. (2) in the case of time-dependent diffusion coefficient for the $\hat{D}=1$, $a=2$, $n=-3/2$, $c_1=1$, $c_2=0$ parameter set and the $t \in [0.1, 1.2]$, $x \in [1, 13]$ domain.

2.3. The case of space-dependent diffusion coefficient

Substituting the first and second derivative of the Ansatz into the original Eq. (2) we arrive to an ordinary differential equation (ODE) for $f(\eta)$

$$-\bar{D}\eta^m f'' + f' \left(\frac{\eta}{s} - \bar{D}m\eta^{m-1} \right) - af = 0$$

if and only if the following constraints hold: a and m are arbitrary real numbers, $b = -1/s$, where $s = m - 2$.

The Maple software again gives the solution of this ODE:

$$f(\eta) = \frac{1}{\sqrt{\eta}} \exp\left(-\frac{\eta^{-s}}{2\bar{D}s^2}\right) \cdot \left\{ c_1 M_{\frac{(1+2sa)|s|}{2s^2}, \frac{m-1}{2s}}\left(\frac{|s|\eta^{-s}}{s^3\bar{D}}\right) + c_2 W_{\frac{(1+2sa)|s|}{2s^2}, \frac{m-1}{2s}}\left(\frac{|s|\eta^{-s}}{s^3\bar{D}}\right) \right\},$$

where M and W are the Whittaker functions [14], [48]. It is worth to mention the formulas for how the Whittaker functions can be expressed [14] in terms of Kummer functions M and U

$$M_{\kappa, \mu}(z) = e^{-1/2z} z^{\mu+1/2} M\left(\mu - \kappa + 1/2, 1 + 2\mu; z\right)$$

$$W_{\kappa, \mu}(z) = e^{-1/2z} z^{\mu+1/2} U\left(\mu - \kappa + 1/2, 1 + 2\mu; z\right)$$

The exponential factor implies that the Whittaker functions have a quicker decay than the Kummer functions. Fig. 3 exemplifies the time development of the concentration function u for a given parameter set.

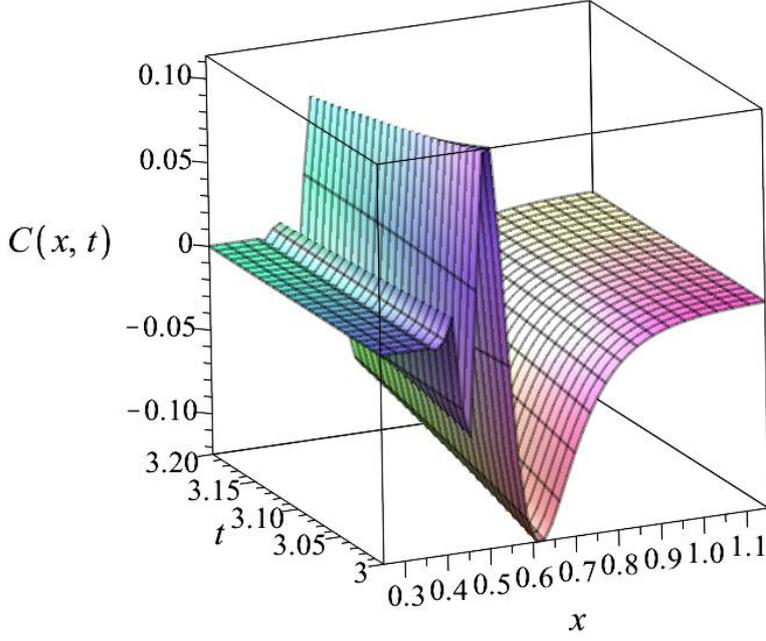


Fig. 3: The solution $u(x, t)$ of Eq. (2) in the case of space-dependent diffusion coefficient for the $\bar{D}=1, a=6, m=10, c_1=0, c_2=1$ parameter set and the $t \in [3, 3.2], x \in [0.25, 1.15]$ domain.

3. The discretization and the numerical schemes

For Eq. (1) and (2) we use the usual central difference operator for the discretization of the second space derivative. In the case of Eq. (3), the material properties depend on space, thus a more general treatment is necessary. We discretize the function $D(x)$ and at the same time the space derivative in Eq. (3) by the standard central difference formula to obtain

$$\frac{du_i}{dt} = \bar{D} \frac{1}{\Delta x} \left(x_{i+1/2}^m \frac{u_{i+1} - u_i}{\Delta x} + x_{i-1/2}^m \frac{u_{i-1} - u_i}{\Delta x} \right)$$

We introduce thermal resistance:

$$R_{i,i+1} = \frac{\Delta x}{\bar{D} x_{i+1/2}^m}$$

with which we obtain the ODE system

$$\frac{du_i}{dt} = \frac{\bar{D}}{\Delta x} \left(\frac{u_{i+1} - u_i}{R_{i,i+1}} + \frac{u_{i-1} - u_i}{R_{i,i-1}} \right),$$

which is the spatially discretized form of Eq. (3). The time variable is always discretized uniformly according to the usual rule:

$$t^j = t^0 + jh, \quad j = 1, \dots, T, \quad hT = t^{\text{fin}} - t^0.$$

The standard definition of the mesh-ratio, $r = \frac{Dh}{\Delta x^2}$ is applicable only for Eq. (1). In case of Eq. (2), D and therefore r is not a constant but changing in time, and must be taken into account always in the proper time point. On the other hand, in the case of Eq. (3) the mesh-ratio is generalized as follows:

$$r_i = \frac{h}{\Delta x} \left(\frac{1}{R_{i,i-1}} + \frac{1}{R_{i,i+1}} \right).$$

We also introduce a brief notation which condense information about the neighbours of the actual cell:

$$A_i = \frac{h}{\Delta x} \left(\frac{u_{i-1}}{R_{i,i-1}} + \frac{u_{i+1}}{R_{i,i+1}} \right).$$

Here some necessary information about the used schemes are briefly presented and the source of the publication are given where the interested reader can find more details. First, the formula of each method is presented for the case of spatially uniform material properties, Eq. (1)). The formulas for Eq. (2) are the same with the difference that the resistances R and therefore the quantities r depend on time and must be recalculated in each time step. After this, the formulas generalized for a non-uniform case (Eq. (3)) are immediately given.

1. The oldest and simplest among our methods is the constant neighbour (CNe) scheme [46], [49]. For Eq. (1) or (2), the following formula must be applied for each node:

$$u_i^{n+1} = u_i^n \cdot e^{-2r} + \frac{u_{i-1}^n + u_{i+1}^n}{2} (1 - e^{-2r}) \quad (6)$$

while for the non-uniform case, the new values of the cell variables are:

$$u_i^{n+1} = u_i^n \cdot e^{-r_i} + \frac{A_i}{r_i} (1 - e^{-r_i})$$

2. The CpC is a two-stage method [44]. The first, predictor stage is a fractional time step with length $\frac{1}{2}h$ with the CNe. The second, corrector stage is full time step size CNe where the predictor values are used to recalculate the A_i quantities.

3. The 2-stage linear-neighbour (LNe or LNe2) method [46]. The first, predictor stage is a full time step CNe. Then the aggregated ‘‘slopes’’ of the neighbours are calculated as

$$s_i = u_{i-1}^{\text{pred}} + u_{i+1}^{\text{pred}} - u_{i-1}^n - u_{i+1}^n.$$

and then, the corrector values of the two-stage LNe method for the uniform case are given as

$$u_i^{n+1} = u_i^n e^{-2r} + \frac{u_{i-1}^n + u_{i+1}^n}{2} (1 - e^{-2r}) + \frac{s_i}{2} \left(1 - \frac{1 - e^{-2r}}{2r} \right) \quad (7)$$

In the non-uniform case, new A_i values must be calculated based on the predictor values. After this the corrector step can be performed based on the formula

$$u_i^{n+1} = u_i^n e^{-r_i} + \left(A_i - \frac{A_i^{\text{new}} - A_i}{r_i} \right) \frac{1 - e^{-r_i}}{r_i} + \frac{A_i^{\text{new}} - A_i}{r_i}. \quad (8)$$

4-5. Based on the obtained corrector values of the LNe scheme, the corrector stage (7) or (8) is repeated. If there is one extra stage (it means three altogether), we have the LNe3 scheme. If there are two extra stages (4 altogether), we call it LNe4 method [46].

6. The CLL method is very similar to LNe3 but with fractional time steps at the first and second stages with $\frac{2}{3}h$, in order to achieve third order temporal convergence [47].

7. The pseudo-implicit (PI) two-stage algorithm [45] applies the θ formula for each node, which can be written as

$$u_i^{n+1} = \frac{(1-2r\theta)u_i^n + r(u_{i-1}^n + u_{i+1}^n)}{1+2r(1-\theta)} \quad \text{and} \quad u_i^{n+1} = \frac{(1-r_i\theta)u_i^n + A_i}{1+r_i(1-\theta)} \quad (9)$$

for the uniform and non-uniform cases, respectively. At the first, predictor stage, a half-sized time step is taken with $\theta = 0$. At the second, corrector stage, a full time step must be taken with $\theta = 1/2$.

For the application of the odd-even hopscotch-type methods, one needs a special, bipartite spatial grid, in which all the nearest neighbors of the odd nodes or cells are even and vice versa. The structure of the examined algorithms are shown in Fig. 4, where the time flows from the top to the down of the figure. In the case of each method, only one odd, and one even cell is present in the figure. The stages are symbolized by colorful boxes while the repeating unit of blocks are surrounded by red dashed line. For example, the leapfrog-hopscotch structure (LH) consists of two half and very many full time steps. First, a half-sized time step (symbolized by a light purple box with the number '0' inside) is taken for the odd cells using the initial values, then full-time steps are taken strictly alternately for the even and odd cells until the end of the last timestep (orange box), which has half-length for odd cells again. One must be aware that when a new value of u_i is calculated, always the latest values of the neighbors $u_{i\pm 1}$ are used, which minimizes the memory usage as well. At points 8-13 we enlist the formulas and indicate if a halved time step size has to be used.

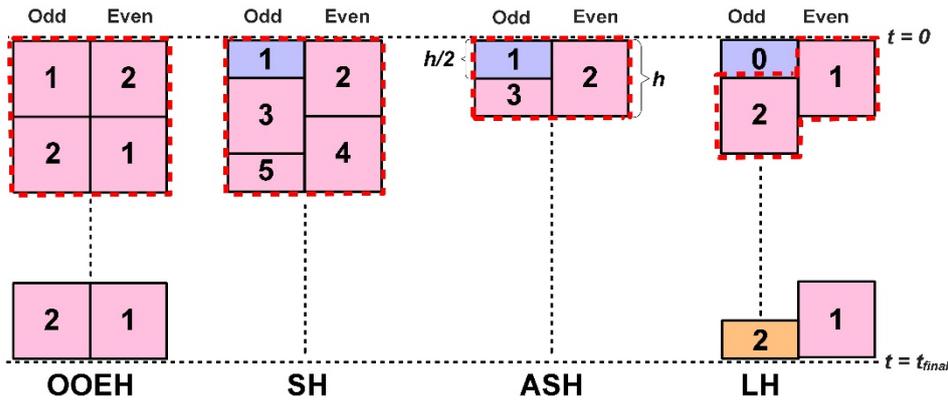


Fig. 4: The structure of the hopscotch-type methods in space and time. From left to right: original odd-even hopscotch (OOEH), shifted-hopscotch (SH), asymmetric hopscotch (ASH), leapfrog-hopscotch (LH). The repeating units are surrounded by thick red dashed line. The formulas of the algorithms are given in the text.

8. Original odd-even hopscotch algorithm (OOEH): stage 1: $\theta = 1$, stage 2: $\theta = 0$.
9. Reversed odd-even hopscotch algorithm (RH): stage 1: $\theta = 0$, stage 2: $\theta = 1$.
10. Shifted-hopscotch (SH): stage 1: $1/2h$, $\theta = 0$. Stages 2-3-4: $\theta = 1/2$, Stage 5: $1/2h$, $\theta = 1$.
11. Asymmetric-hopscotch (ASH): Stage 1: $1/2h$, $\theta = 0$. Stage 2: $\theta = 1/2$, Stage 3: $1/2h$, $\theta = 1$.
12. Leapfrog-hopscotch (LH): Stage 0: $1/2h$, $\theta = 0$. Intermediate stages: $\theta = 1/2$, Last stage: $1/2h$, $\theta = 1/2$.
13. Leapfrog-hopscotch-CNe (LH-CNe): Same structure as LH, but always the CNe formula with the appropriate time step size.

14. The FTCS (the standard Forward-time Central-space) scheme is actually the θ formula (9) for $\theta = 1$.

15. The Dufort-Frankel (DF) is a known 1-stage but 2-step algorithm

$$u_i^{n+1} = \frac{(1-2r)u_i^{n-1} + 2r(u_{i-1}^n + u_{i+1}^n)}{1+2r} \quad \text{and} \quad u_i^{n+1} = \frac{(1-r_i)u_i^{n-1} + 2A_i}{1+r_i}.$$

The CNe scheme is used for the starting time step.

16. The alternating direction explicit (ADE) scheme is a known method. It is explicit only for the uniform case, so we do not apply it to Eq. (3). One must split the calculations based on the directions: when one moves from left to right, the variable is denoted by p , and when from right to left, it is denoted by q (both has to be initialized similarly to u). The formulas are the following:

$$p_i^{n+1} = \frac{(1-r)p_i^n + r(p_{i-1}^{n+1} + p_{i+1}^n)}{1+r} \quad \text{and} \quad q_i^{n+1} = \frac{(1-r)q_i^n + r(q_{i-1}^n + q_{i+1}^{n+1})}{1+r}.$$

and then average $u_i^{n+1} = (p_i^{n+1} + q_i^{n+1})/2$ gives the solution for each node. It uses the new values of the neighbours p_{i-1}^{n+1} and q_{i+1}^{n+1} , thus it cannot be parallelized so straightforwardly.

The CNe, CpC, LNe, LNe3-4, CLL, LH-CNe, LH, RH, SH, ASH, and PI methods are constructed by our research group. CNe and FTCS has first order convergence, CLL third order, all others have second order. All of the examined methods, except the FTCS, are unconditionally stable in the case of Eqs. (1)-(3), there is no CFL limit. The CNe, CpC, LNe, LNe3-4, and the LH-CNe has dynamical consistency (the new values are the convex combination of the old values). It implies that the Maximum and Minimum principles are automatically fulfilled.

4. The numerical results

All the simulations are performed in a MATLAB environment. For several fixed time step sizes, we are going to calculate the error of each method, which means we compare the numerical and the analytical solution node by node and select the difference with the maximum absolute value.

4.1. The case of constant diffusion coefficient

We reproduce the solution (5), under the circumstances presented in Fig. 1. It means $D = 1$, $t \in [0.1, 0.2]$, $x \in [0, 3]$, and $\Delta x = 0.01$. In Fig. 5 the errors of the examined methods as a function of the time step size are presented in a log-log diagram. The calculated CFL limit for the FTCS scheme is $5 \cdot 10^{-5}$. Indeed, that scheme gives meaningful result only below this limit, but all of the unconditionally stable methods are usable above this.

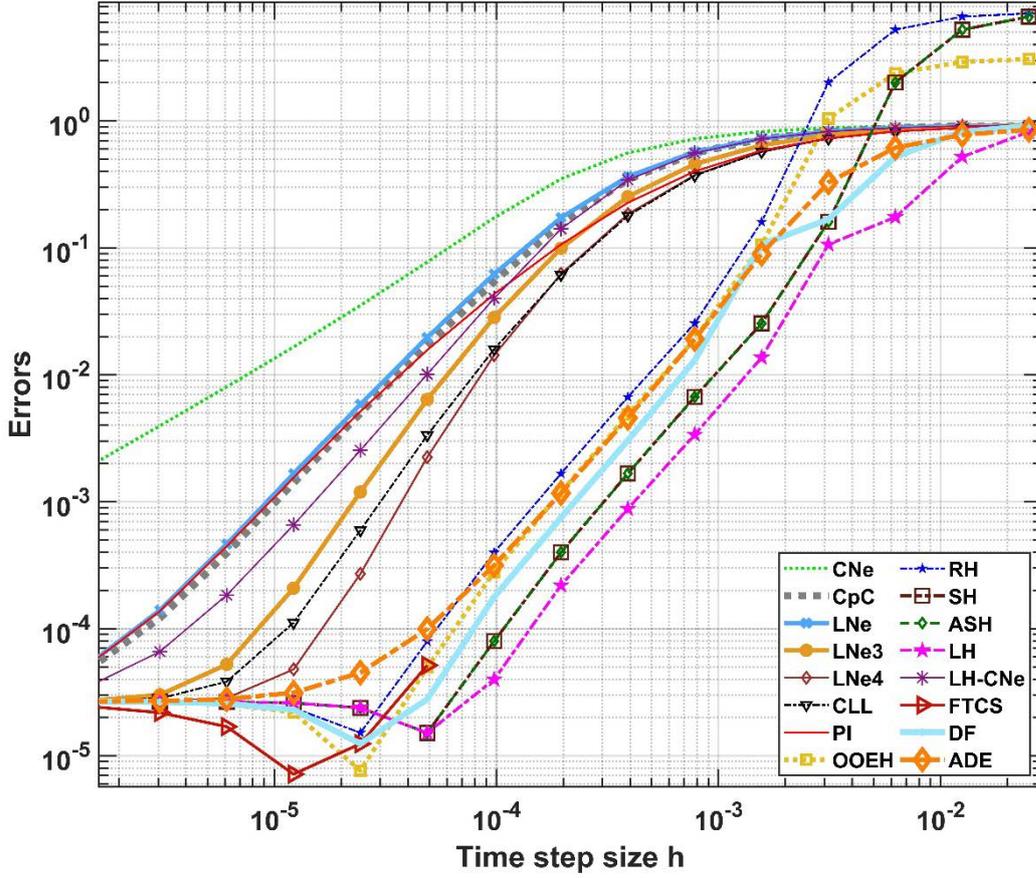


Fig. 5: Errors as a function of the effective time step size h for constant diffusion coefficient. The slope of the error-curves show the temporal order of convergence of the methods.

4.2. The case of time-dependent diffusion coefficient

We reproduce the solution presented in Fig. 2, so $\hat{D}=1$, $a=2$, $n=-\frac{3}{2}$, $c_1=1$, $c_2=0$, $t \in [0.1, 1.2]$, $x \in [1, 13]$ and $\Delta x=0.05$. In Fig. 6 the errors of the examined methods as a function of the time step size are presented. The calculated CFL limit for the FTCS scheme is increasing from $6.3 \cdot 10^{-6}$ to $1.8 \cdot 10^{-5}$. Below $h=6.3 \cdot 10^{-6}$, the FTCS scheme is very accurate. However, the other algorithms are more reliable and able to reproduce the exploding solution without any instability issues.

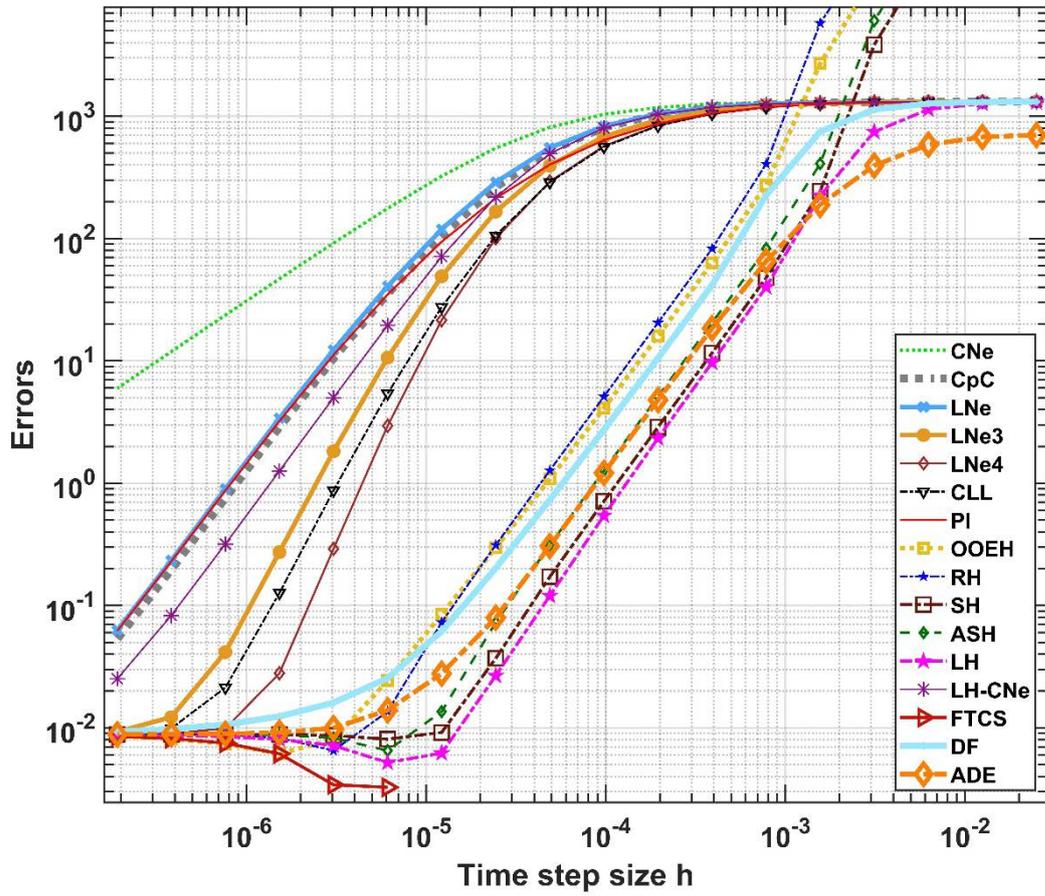


Fig. 6: Errors as a function of the effective time step size h in the case of the exploding solution when the diffusion coefficient depends on time.

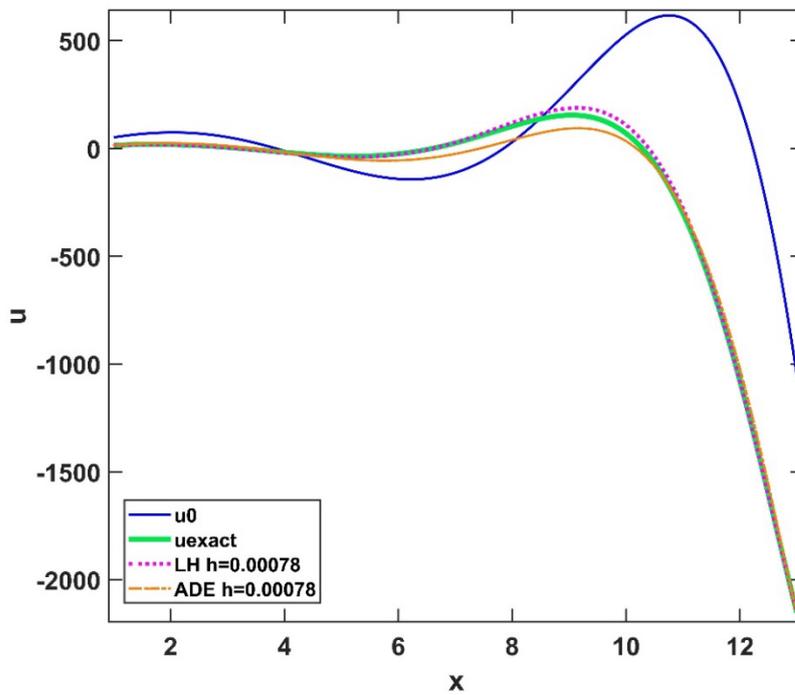


Fig. 7: The concentration u as a function of the x variable in the case of the initial function u^0 , the analytical solution at t^{fin} , and two numerical solutions for the case of the time-dependent diffusion coefficient. We underline that the standard Runge-Kutta methods are unstable for these time step sizes.

4.3. The case of space-dependent diffusion coefficient

We reproduce the solution of Fig. 3, which means $\bar{D}=1$, $a=6$, $m=10$, $c_1=0$, $c_2=1$, $t \in [3, 3.2]$, $x \in [0.25, 1.15]$. We use a very small space step size, namely $\Delta x = 0.0005$. The calculated CFL limit for the FTCS scheme is $3.2 \cdot 10^{-8}$. Due to this, the FTCS scheme did not give any result, it was unstable for all the used time step sizes, unlike the unconditionally stable explicit methods.

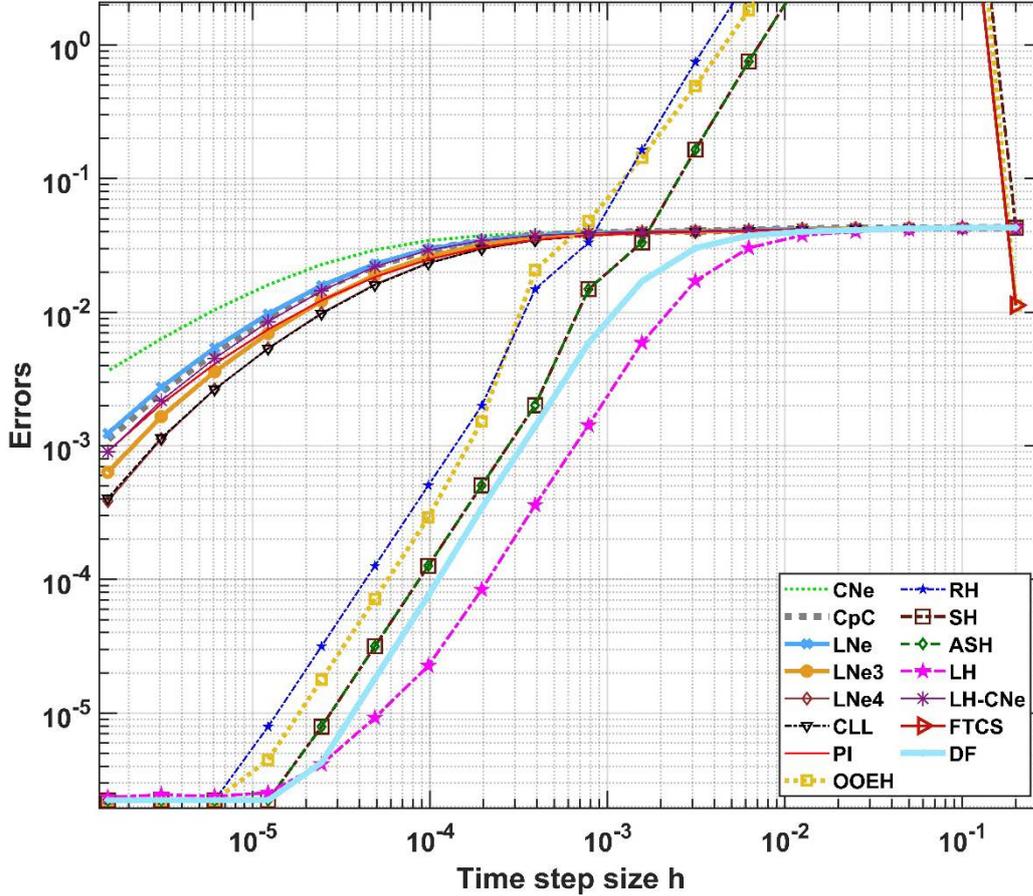


Fig. 8: Errors as a function of the effective time step size h in the case of the space-dependent diffusion coefficient. The used parameters and the domain are the same as in Fig. 3, but the space step size is quite small: $\Delta x = 0.0005$.

3. Conclusions

We have constructed a set of analytical solutions for the one dimensional regular diffusion equation when the diffusion coefficient depends on time or the spatial coordinate using a similarity transform. The derived solutions can be expressed with Kummer's or the Whittaker functions which are highly nontrivial results.

We reproduced the presented analytical solutions by 16 numerical methods (15 in the case of the space-dependent diffusion coefficient). One of these methods is the most standard FTCS scheme, and the others are explicit and unconditionally stable schemes. Three members of this latter group is known for decades, but the others are recently invented. We observed that the leapfrog-hopscotch algorithm has the best performance in all cases for almost all time step sizes. For medium and small time step sizes, some other hopscotch-type methods also perform well, and the Dufort-Frankel scheme is quite competitive, too. If the CFL limit is very small, even

the least accurate CNe method can outperform the FTCS scheme. It can be generally stated that it is better to use the unconditionally stable explicit methods than the conditionally stable traditional ones for these kinds of problems.

References

- [1] M. M. Hefny and A. M. Tawfik, “The Fate of Molecular Species in Water Layers in the Light of Power-Law Time-Dependent Diffusion Coefficient,” *Symmetry (Basel)*, vol. 14, no. 6, p. 1146, Jun. 2022, doi: 10.3390/sym14061146.
- [2] M. H. Jacobs, *Diffusion Processes*. Springer Berlin Heidelberg, 1935.
- [3] D. Reguera and J. M. Rubí, “Kinetic equations for diffusion in the presence of entropic barriers,” *Phys. Rev. E - Stat. Physics, Plasmas, Fluids, Relat. Interdiscip. Top.*, vol. 64, no. 6, p. 8, Nov. 2001, doi: 10.1103/PhysRevE.64.061106.
- [4] R. Zwanzig, “Diffusion past an entropy barrier,” *J. Phys. Chem.*, vol. 96, no. 10, pp. 3926–3930, 1992, doi: 10.1021/j100189a004.
- [5] M. Wolfson, C. Liepold, B. Lin, and S. A. Rice, “A comment on the position dependent diffusion coefficient representation of structural heterogeneity,” *J. Chem. Phys.*, vol. 148, no. 19, p. 194901, May 2018, doi: 10.1063/1.5025921.
- [6] A. Berezhkovskii and G. Hummer, “Single-file transport of water molecules through a carbon nanotube,” *Phys. Rev. Lett.*, vol. 89, no. 6, pp. 064503/1-064503/4, Aug. 2002, doi: 10.1103/PhysRevLett.89.064503.
- [7] B. Hille, *Ion Channels of Excitable Membranes (3rd Edition)*, 3rd ed. New York: Oxford University Press Inc, 2001.
- [8] J. Kärger and D. M. Ruthven, *Diffusion in Zeolites and other Microporous Solids*. New York: Wiley, 1992.
- [9] L. Mátyás and I. F. Barna, “General Self-Similar Solutions of Diffusion Equation and Related Constructions,” *Rom. J. Phys.*, vol. 67, p. 101, 2022.
- [10] I. F. Barna and L. Mátyás, “Advanced Analytic Self-Similar Solutions of Regular and Irregular Diffusion Equations,” *Mathematics*, vol. 10, no. 18, p. 3281, Sep. 2022, doi: 10.3390/math10183281.
- [11] G. Bluman and J. Cole, “The General Similarity Solution of the Heat Equation,” *J. Math. Mech.*, vol. 18, no. 11, pp. 1025–1042, 1969.
- [12] C. Zoppou and J. H. Knight, “Analytical solution of a spatially variable coefficient advection-diffusion equation in up to three dimensions,” *Appl. Math. Model.*, vol. 23, no. 9, pp. 667–685, 1999, doi: 10.1016/S0307-904X(99)00005-0.
- [13] I. F. Barna, “Self-similar solutions of three-dimensional Navier - Stokes equation,” *Commun. Theor. Phys.*, vol. 56, no. 4, pp. 745–750, Oct. 2011, doi: 10.1088/0253-6102/56/4/25.
- [14] F.W.J. Olver, D.W. Lozier, R.F. Boisvert, and C.W. Clark, *NIST Handbook of Mathematical Functions*, vol. 66, no. 1. New York: Cambridge Univ. Press, 2011.
- [15] I. F. Barna and L. Mátyás, “Analytic solutions for the three-dimensional compressible Navier-Stokes equation,” *Fluid Dyn. Res.*, vol. 46, no. 5, p. 055508, Oct. 2014, doi: 10.1088/0169-5983/46/5/055508.
- [16] Á. Nagy, I. Omle, H. Kareem, E. Kovács, I. F. Barna, and G. Bogнар, “Stable, Explicit, Leapfrog-Hopscotch Algorithms for the Diffusion Equation,” *Computation*, vol. 9, no. 8, p. 92, 2021.
- [17] S. M. Savović and A. Djordjevich, “Numerical solution of diffusion equation describing the flow of radon through concrete,” *Appl. Radiat. Isot.*, vol. 66, no. 4, pp. 552–555, 2008, doi: 10.1016/j.apradiso.2007.08.018.
- [18] F. Suárez-Carreño and L. Rosales-Romero, “Convergency and stability of explicit and implicit schemes in the simulation of the heat equation,” *Appl. Sci.*, vol. 11, no. 10, 2021,

- doi: 10.3390/app11104468.
- [19] S. A. Lima, M. Kamrujjaman, and M. S. Islam, “Numerical solution of convection-diffusion-reaction equations by a finite element method with error correlation,” *AIP Adv.*, vol. 11, no. 8, pp. 1–12, 2021, doi: 10.1063/5.0050792.
 - [20] V. Kumar, K. Chandan, K. V. Nagaraja, and M. V. Reddy, “Heat Conduction with Krylov Subspace Method Using FEniCSx,” *Energies*, vol. 15, no. 21, p. 8077, Oct. 2022, doi: 10.3390/en15218077.
 - [21] M. Ivanovic, M. Svicevic, and S. Savovic, “Numerical solution of Stefan problem with variable space grid method based on mixed finite element/ finite difference approach,” *Int. J. Numer. Methods Heat Fluid Flow*, vol. 27, no. 12, pp. 2682–2695, 2017, doi: 10.1108/HFF-02-2014-0034.
 - [22] P. O. Appau, O. K. Dankwa, and E. T. Brantson, “A comparative study between finite difference explicit and implicit method for predicting pressure distribution in a petroleum reservoir,” *Int. J. Eng. Sci. Technol.*, vol. 11, no. 4, 2019, doi: 10.4314/ijest.v11i4.3.
 - [23] A. Moncorgé, H. A. Tchelepi, and P. Jenny, “Modified sequential fully implicit scheme for compositional flow simulation,” *J. Comput. Phys.*, vol. 337, no. 15, pp. 98–115, 2017, doi: 10.1016/j.jcp.2017.02.032.
 - [24] C. S. Chou, Y. T. Zhang, R. Zhao, and Q. Nie, “Numerical methods for stiff reaction-diffusion systems,” *Discret. Contin. Dyn. Syst. - Ser. B*, vol. 7, no. 3, pp. 515–525, 2007, doi: 10.3934/dcdsb.2007.7.515.
 - [25] J. Zhang and C. Zhao, “Sharp error estimate of BDF2 scheme with variable time steps for molecular beam epitaxial models without slope selection,” *J. Math.*, vol. 41, no. 6, pp. 1–19, 2021.
 - [26] J. Amoah-mensah, F. O. Boateng, and K. Bonsu, “Numerical solution to parabolic PDE using implicit finite difference approach,” *Math. Theory Model.*, vol. 6, no. 8, pp. 74–84, 2016.
 - [27] N. A. Mbroh and J. B. Munyakazi, “A robust numerical scheme for singularly perturbed parabolic reaction-diffusion problems via the method of lines,” *Int. J. Comput. Math.*, no. May, 2021, doi: 10.1080/00207160.2021.1954621.
 - [28] H. Aminikhah and J. Alavi, “An efficient B-spline difference method for solving system of nonlinear parabolic PDEs,” *SeMA J.*, vol. 75, no. 2, pp. 335–348, 2018, doi: 10.1007/s40324-017-0139-8.
 - [29] I. Ali, S. Haq, K. S. Nisar, and S. U. Arifeen, “Numerical study of 1D and 2D advection-diffusion-reaction equations using Lucas and Fibonacci polynomials,” *Arab. J. Math.*, 2021, doi: 10.1007/s40065-021-00330-4.
 - [30] M. K. Singh, S. Rajput, and R. K. Singh, “Study of 2D contaminant transport with depth varying input source in a groundwater reservoir,” *Water Sci. Technol. Water Supply*, vol. 21, no. 4, pp. 1464–1480, 2021, doi: 10.2166/WS.2021.010.
 - [31] Y. Ji, H. Zhang, and Y. Xing, “New Insights into a Three-Sub-Step Composite Method and Its Performance on Multibody Systems,” *Mathematics*, vol. 10, no. 14, p. 2375, Jul. 2022, doi: 10.3390/math10142375.
 - [32] A. R. Appadu, “Performance of UPFD scheme under some different regimes of advection, diffusion and reaction,” *Int. J. Numer. Methods Heat Fluid Flow*, vol. 27, no. 7, pp. 1412–1429, 2017, doi: 10.1108/HFF-01-2016-0038.
 - [33] H. Karahan, “Unconditional stable explicit finite difference technique for the advection-diffusion equation using spreadsheets,” *Adv. Eng. Softw.*, vol. 38, no. 2, pp. 80–86, 2007, doi: 10.1016/j.advengsoft.2006.08.001.
 - [34] F. Sanjaya and S. Mungkasi, “A simple but accurate explicit finite difference method for the advection-diffusion equation,” *J. Phys. Conf. Ser.*, vol. 909, no. 1, pp. 1–5, 2017, doi: 10.1088/1742-6596/909/1/012038.

- [35] S. Pourghanbar, J. Manafian, M. Ranjbar, A. Aliyeva, and Y. S. Gasimov, “An efficient alternating direction explicit method for solving a nonlinear partial differential equation,” *Math. Probl. Eng.*, vol. 2020, no. November, pp. 1–12, 2020, doi: 10.1155/2020/9647416.
- [36] A. Al-Bayati, S. Manaa, and A. Al-Rozbayani, “Comparison of Finite Difference Solution Methods for Reaction Diffusion System in Two Dimensions,” *AL-Rafidain J. Comput. Sci. Math.*, vol. 8, no. 1, pp. 21–36, 2011, doi: 10.33899/csmj.2011.163605.
- [37] C. Nwaigwe, “An Unconditionally Stable Scheme for Two-Dimensional Convection-Diffusion-Reaction Equations,” no. January, 2022.
- [38] S. Savović, B. Drljača, and A. Djordjevich, “A comparative study of two different finite difference methods for solving advection–diffusion reaction equation for modeling exponential traveling wave in heat and mass transfer processes,” *Ric. di Mat.*, vol. 71, pp. 245–252, 2022, doi: 10.1007/s11587-021-00665-2.
- [39] Q. A. Dang and M. T. Hoang, “Positive and elementary stable explicit nonstandard Runge-Kutta methods for a class of autonomous dynamical systems,” *Int. J. Comput. Math.*, vol. 97, no. 10, pp. 2036–2054, Oct. 2020, doi: 10.1080/00207160.2019.1677895.
- [40] M. Saleh, Á. Nagy, and E. Kovács, “Part 1: Construction and investigation of new numerical algorithms for the heat equation,” *Multidiszcip. tudományok*, vol. 10, no. 4, pp. 323–338, 2020, doi: 10.35925/j.multi.2020.4.36.
- [41] M. Saleh, Á. Nagy, and E. Kovács, “Part 2: Construction and investigation of new numerical algorithms for the heat equation,” *Multidiszcip. tudományok*, vol. 10, no. 4, pp. 339–348, 2020, doi: 10.35925/j.multi.2020.4.37.
- [42] M. Saleh, Á. Nagy, and E. Kovács, “Part 3: Construction and investigation of new numerical algorithms for the heat equation,” *Multidiszcip. tudományok*, vol. 10, no. 4, pp. 349–360, 2020, doi: 10.35925/j.multi.2020.4.38.
- [43] Á. Nagy, M. Saleh, I. Omle, H. Kareem, and E. Kovács, “New stable, explicit, shifted-hopscotch algorithms for the heat equation,” *Math. Comput. Appl.*, vol. 26, no. 61, 2021.
- [44] E. Kovács, Á. Nagy, and M. Saleh, “A set of new stable, explicit, second order schemes for the non-stationary heat conduction equation,” *Mathematics*, vol. 9, no. 18, p. 2284, Sep. 2021, doi: 10.3390/math9182284.
- [45] H. K. Jalghaf, E. Kovács, J. Majár, Á. Nagy, and A. H. Askar, “Explicit stable finite difference methods for diffusion-reaction type equations,” *Mathematics*, vol. 9, no. 24, 2021, doi: 10.3390/math9243308.
- [46] E. Kovács, “A class of new stable, explicit methods to solve the non-stationary heat equation,” *Numer. Methods Partial Differ. Equ.*, vol. 37, no. 3, pp. 2469–2489, 2020, doi: 10.1002/num.22730.
- [47] E. Kovács, Á. Nagy, and M. Saleh, “A New Stable, Explicit, Third-Order Method for Diffusion-Type Problems,” *Adv. Theory Simulations*, 2022, doi: 10.1002/adts.202100600.
- [48] Wikipedia, “Whittaker function.” [Online]. Available: https://en.wikipedia.org/wiki/Whittaker_function.
- [49] E. Kovács, “New Stable, Explicit, First Order Method to Solve the Heat Conduction Equation,” *J. Comput. Appl. Mech.*, vol. 15, no. 1, pp. 3–13, 2020, doi: 10.32973/jcam.2020.001.