SCIENTIA PLENA
www.scientiaplena.org.br
VOL. 19, NUM. 11 2023
doi: 10.14808/sci.plena.2023.119901

Numerical solution of the Fokker-Planck Equation using Orthogonal Collocation

Resolução numérica da Equação de Fokker-Planck usando Colocação Ortogonal

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(Recebido em 04 de janeiro de 2023; aceito em 14 de agosto de 2023)

This study aims to propose a numerical methodology to solve the Fokker-Planck Equation using the Orthogonal Collocation Method. In this approach, the original problem, represented by a partial differential equation, is rewritten as a system of initial value equations via discretization of spatial variable. The resulting system is integrated considering the Runge-Kutta-Fehlberg Method. The proposed methodology is applied in three case studies that presented an analytical solution. The obtained results demonstrate that the proposed approach is a good alternative for solving this class of problems.
Keywords: fokker-planck equation, orthogonal collocation, numerical method.

Este trabalho tem por objetivo propor uma metodologia para a resolução numérica da Equação de Fokker-Planck usando o Método da Colocação Ortogonal. Nesta abordagem, o problema original, representado por uma equação diferencial parcial, é reescrito como um sistema de equações de valor inicial via discretização da variável espacial. O sistema resultante é integrado considerando o Método de Runge-Kutta-Fehlberg. A metodologia proposta é aplicada em três estudos de caso que apresentam solução analítica. Os resultados obtidos demonstram que a abordagem proposta se configura uma boa alternativa para a resolução desta classe de problemas.
Palavras-chave: equação de fokker-planck, colocação ortogonal, método numérico.

1. INTRODUCTION

The Fokker-Planck Equation (FPE) was developed to describe the Brownian motion of particles, represent the variation of probability of a random function in space and time, and study stochastic processes [1]. As mentioned by Liu et al. (2021) [2], during a stochastic process, the temporal evolution of variables is affected by random fluctuations. As a consequence, it is impossible to obtain a deterministic trajectory. Thus, the randomness can be characterized by using a probability density function in relation to random variable. In the literature, various applications involving the FPE in different field of science can be found [1,3-7].

In practice, the analytical solution of this equation can only be obtained for very particular situations. Thus, numerical methods should be used to obtain the profiles that characterize a given case study. In this scenario, Chang and Cooper (1970) [3] proposed a so-called Chang-Cooper scheme to solve the FPE, in which one of its main advantages is the fact that this scheme preserves characteristics as positivity and conservation of total probability of the original problem. In this same context, schemes based on finite elements [4] can also be found. Tatari et al. (2007) [5] and Biazar (2010) [8] employed the Variational Iteration Method to solve this equation. In a stochastic context, we can cite the development of a discretization scheme developed by Carlini and Silva (2018) [6] to solve the PFE. In this case, the non-negativity of the solution and conservation of mass are preserved. Harrison (1988) [9] developed a moving finite element method to solve the FPE. Dehghan and Tatari (2006) [10] applied the Adomian Decomposition Method to solve the FPE. Fasshauer (2007) [11] proposed meshfree approximation methods to solve the FPE with different characteristics. Jafari and Aminataei (2009) [12] evaluated the application of a homotopy perturbation method in the solution of this equation. Lakestani and Dehghan (2009) [13] proposed a numerical approach based on cubic splines to reduce the original problem (partial differential) to a set of algebraic equations. Pichler (2013) [14] evaluated both the Finite Difference Method

and the Finite Element Method for solving the FPE. In a similar way, Sepehrian and Radpoor (2015) [15] proposed a Finite Difference scheme associated with the Spline Cubic Collocation Method for solving the non-linear FPE. In a fractional context, the FPE was solved by using the Spectral Method [16].

In this contribution, the aim is to propose a systematic methodology for solving the FPE considering the Orthogonal Collocation Method (OCM).

2. FOKKER-PLANCK EQUATION

In this contribution, the FPE is used to represent the concentration field $u(x,t)$ in function of time t and a spatial variable x [1,5,6,9,11,13]. Mathematically, this model is given by the following equation:

$$\frac{\partial u(x,t)}{\partial t} = \left[-A(x,t)\frac{\partial}{\partial x} + B(x,t)\frac{\partial^2}{\partial x^2} \right] u(x,t) \tag{1}$$

The initial condition is described by thefollowing relation:

$$u(x,0) = f(x) \tag{2}$$

In this model, B is the diffusion coefficient, A is the drift coefficient and $f(x)$ is a function that characterizes the initial condition associated with the variable u at t equal to zero. From the mathematical point of view, this model is a parabolic second-order linear partial differential equation, also known as the direct Kolmogorov equation [1].

According to Biazar (2010) [11], the general form of the FPE presents nonlinearities. This is to capture the phenomena observed in different areas of science. In this case, the nonlinear FPE is given as:

$$\frac{\partial u(x,t)}{\partial t} = \left[-A(x,t,u)\frac{\partial}{\partial x} + B(x,t,u)\frac{\partial^2}{\partial x^2} \right] u(x,t) \tag{3}$$

where the initial condition is given by:

$$u(x,0) = f(x) \tag{4}$$

In this work, the terms $A(x,t,u)$, $B(x,t,u)$ and $f(x)$ will be chosen to represent three particular cases considered to describe systems of interest for validating the proposed methodology.

3. METHODOLOGY

In this study, to solve the FPE the Orthogonal Collocation Method (OCM) is used. This numerical strategy evaluate collocation (discretized) points inside the domain of interest X (Number of Collocation Points - *NCP*) by using a polynomial function [17]. It is important to mention that the boundary conditions should be satisfied. The polynomial approximation is obtained by using the following recursive relation [17]:

$$\Gamma_i^{(\psi,\eta)}(X) = (X + \psi_i)\Gamma_{i-1}(X) + \eta_i \Gamma_{i-2}(X) \tag{5}$$

where Γ_{i-1}, Γ_{i-2}, ψ, and η are parameters that depends of polynomial approximation.

The roots (collocation points) are obtained by using an orthogonal polynomial of degree *NCP* and weight $W(X)$ together with the Galerkin condition [17]:

$$\int_0^1 W(X)(\psi X + \eta)\Gamma_i^{(\psi,\eta)}(X)\,dX = 0, \quad i = 0,\ ...,\ NCP - 2 \tag{6}$$

Multiplying Eq.(5) by Γ_{i-2}, the following expression is obtained:

$$\eta_i = -\frac{\int_0^1 XW(X)\Gamma_{i-1}(X)\Gamma_{i-2}(X)dX}{\int_0^1 W(X)\Gamma_{i-2}^2(X)dX} \tag{7}$$

Similarly, multiplying Eq.(5) by Γ_{i-1}, ψ is determined:

$$\psi_i = -\frac{\int_0^1 XW(X)\Gamma_{i-1}^2(X)dX}{\int_0^1 W(X)\Gamma_{i-1}^2(X)dX} \tag{8}$$

If Γ_{i-2}, Γ_{i-1}, $W(X)$ and η_1 are known, ψ and η can be estimated and the proposed polynomial approximation ($\Gamma_{NCP}^{(\psi,\eta)}(X)$) can be evaluated [17].

The Lagrange Polynomial (LP) is used as approximation function. It is due to reduction of the computational cost necessary to determine the derivatives [17]. Thus, consider the set of data points (X_1, Y_1), (X_2, Y_2), …, (X_{NCP+1}, Y_{NCP+1}) and an interpolation formula passing through these points (an *NCP*-th degree interpolation polynomial), as follows:

$$Y_{NCP}(X) = \sum_{i=1}^{NCP+1} Y_i l_i(X) \tag{9}$$

where $l_i(X)$ is the Lagrange interpolation polynomial, computed as:

$$l_i(X) = \prod_{j=1}^{NCP+1} \frac{X - X_j}{X_i - X_j} \tag{10}$$

where $l_i(X)$ is equal to 1 if i is equal to j, and equal to 0 otherwise. The first derivative evaluate at X_j is computed as:

$$\frac{dY_{NCP}(X_j)}{dX} = \sum_{i=1}^{NCP+1} Y_i \frac{dl_i(X_j)}{dX}, \quad j = 1,2,...,NCP+1 \tag{11}$$

In this case, the polynomial approximation is computed as:

$$x(t) = \sum_{i=1}^{NCP} l_i \phi_i(t) \tag{12}$$

where ϕ depends on time t. Thus, if x is replaced in the original model, a system of ordinary differential equations at i-th root (collocation points) is formed.

In summary, the proposed OCM is characterized as follows [17,18]:

- Define the input parameters: mathematical model, initial and boundary conditions, order (N) of approximation, and the type of orthogonal polynomial to determine the collocation points.
- Determine the collocation points (roots of the orthogonal polynomial).
- Generate the LP orthogonal polynomial by using the collocation points.
- Replace the approximation function in the original model. In this case, the model original is transformed into an equivalent formed by ordinary differential equations where the boundary conditions are satisfied.
- Solve this model considering a specific solver.
- Evaluate the influence of solution in relation to number of collocation points.

4. RESULTS AND DISCUSSION

In each application, the proposed models by Tatari et al. (2007) [5] and Dehghan and Tatari (2006) [10] and solved by Lakestani and Dehghan (2009) [13] using Cubic B-Spline Scaling Functions are considered. Thus, each boundary condition is defined from the evaluation of analytical solution in x equal to zero and x equal to unity.

After applying the OCM, a system with $NCP \times 50$ initial value ordinary differential equations are obtained (where 50 is the number of discretization points in the temporal coordinate, defined after preliminary simulations). To solve this system, the Runge-Kutta-Fehlberg is used).

To evaluate the processing time (PT), an Intel Core i7-4770 Desktop microcomputer with 8GB of memory is considered.

4.1 Case Study 1

The first case study considers $A(x,t)=-1$, $B(x,t)=1$ and $f(x)=x$ in Eq.(1)-(2). For these parameters, the analytical solution is $u(x,t)=x+t$. Table 1 presents the absolute errors considering the influence of *NCP* for the first case study, where both the solutions (numerical and analytical) are evaluated at x = [0.2 0.4 0.6 0.8] and for t equal to unity.

Table 1: Absolute error computed for the first case study considering different values for NCP ([2 3 4 5]), x ([0.2 0.4 0.6 0.8]) and t is equal to unity.

NCP	***x*=0.2**	***x*=0.4**	***x*=0.6**	***x*=0.8**	**PT (s)**
2	1.7344×10^{-6}	7.3434×10^{-6}	4.3455×10^{-5}	6.6787×10^{-6}	0.0311
3	1.3556×10^{-6}	2.5699×10^{-6}	1.5666×10^{-6}	2.6887×10^{-6}	0.0544
4	6.8778×10^{-8}	7.987×10^{-8}	5.7711×10^{-8}	3.8678×10^{-8}	0.1442
5	4.4574×10^{-9}	7.9401×10^{-9}	4.1656×10^{-9}	3.0671×10^{-9}	0.7489

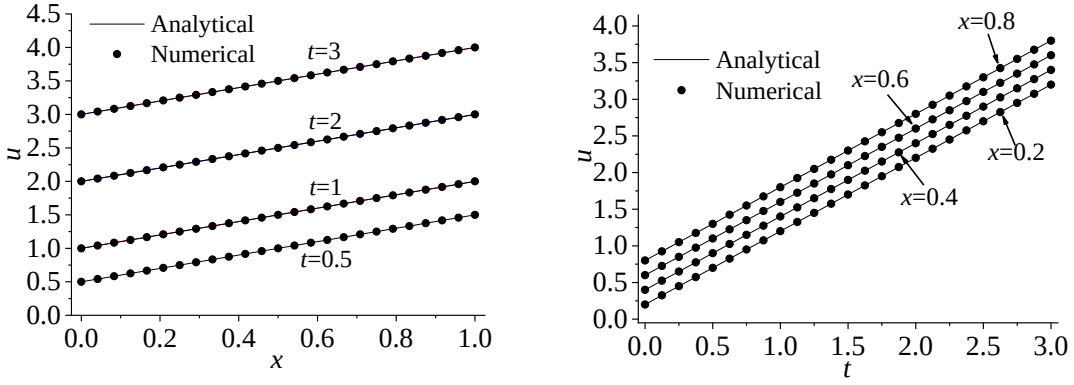
Table 1 shows that the increase in the value of the parameter *NCP* implies in increasing the accuracy of the proposed methodology. This result is expected as the increase in value of the number of collocation points implies an ordinary differential system with a greater number of equations, which in practice means a greater refinement of the proposed numerical solution. As a consequence, the processing time increases with the increment of *NCP*.

It should be noted that the obtained results are in agreement with those reported by Lakestani and Dehghan (2009) [13] for *NCP* equal to 2, as the absolute error is, approximately, equal to 10^{-6} in t equal to unity. For larger values of *NCP*, the absolute errors computed considering the proposed methodology are smaller than those reported by Lakestani and Dehghan (2009) [13].

Figures 1a and 1b presents the comparison between analytical and numerical profiles for the dependent variable u in relation to independent variables, respectively. For this purpose, *NCP* is considered equal to 5, as well as the respective analytical solutions for t = [0.5 1 2 3] and x = [0.2 0.4 0.6 0.8]. In these figures, it can be seen that the OCM was able to obtain good estimates for all profiles in relation to the respective analytical solutions.

4.2 Case Study 2

This case study considers $A(x,t)=-x$, $B(x,t)=0.5x^2$ and $f(x)=x$ in Eq.(1)-(2). These inputs corresponds to analytical solution $u(x,t)=xe^t$. Table 2 presents the absolute errors considering the influence of *NCP* for the second case study considering numerical and analytical solutions at x = [0.2 0.4 0.6 0.8] and for t equal to unity.



(a) $u \times x$. (b) $u \times t$.

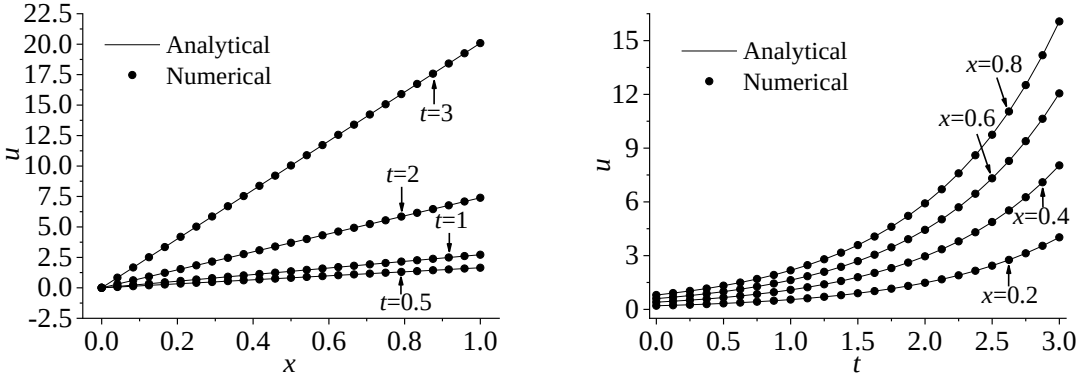
Figure 1: Analytical versus numerical profiles for the first case study.

Table2: Absolute error computed for the second case study considering different values for NCP ([2 3 4 5]), x ([0.2 0.4 0.6 0.8]) and t is equal to unity.

NCP	***x*=0.2**	***x*=0.4**	***x*=0.6**	***x*=0.8**	**PT (s)**
2	9.4345×10^{-6}	8.9896×10^{-6}	9.4645×10^{-6}	7.3544×10^{-6}	0.0112
3	2.4544×10^{-6}	3.5455×10^{-7}	4.4444×10^{-7}	1.4678×10^{-6}	0.0543
4	3.4999×10^{-8}	3.8987×10^{-8}	6.7878×10^{-8}	6.6667×10^{-8}	0.3455
5	2.7144×10^{-9}	2.1676×10^{-9}	3.1345×10^{-9}	6.7881×10^{-9}	0.8954

In this table, it can be concluded that, as expected, the increase of *NCP* implies in increase in theaccuracy of the proposed approach. Therefore, the processing time is proportional to the value of *NCP*, i.e., an increment in the value of this parameter implies in an increase in PT. The obtained results are in agreement with those obtained by Lakestani and Dehghan (2009) [13] for *NCP* equal to 3, i.e., absolute errors of order of 10^{-7} in *t* equal to unity are observed. For larger values of *NCP*, the absolute errors computed considering the proposed methodology are similar to those reported by Lakestani and Dehghan (2009) [13].

Figures 2a and 2b shows the dependent variable profiles considering *NCP* equal to 5, t = [0.5 1 2 3] and x = [0.2 0.4 0.6 0.8]. As observed for the first application, the proposed methodology was able to obtain good estimates for all profiles in relation to the analytical solutions.



(a) $u \times x$. (b) $u \times t$.

Figure 2: Analytical versus numerical profiles for the second case study.

4.3 Case Study 3

The last case considers $A(x,t)=-(x+1)$, $B(x,t)=x^2e^t$ and $f(x)=x+1$ in Eq.(1)-(2). The analytical solution for these inputs is $u(x,t)=(x+1)e^t$. Table 3 presents the absolute errors considering the influence of *NCP* for the second case study considering numerical and analytical solutions at x = [0.2 0.4 0.6 0.8] and for t equal to unity.

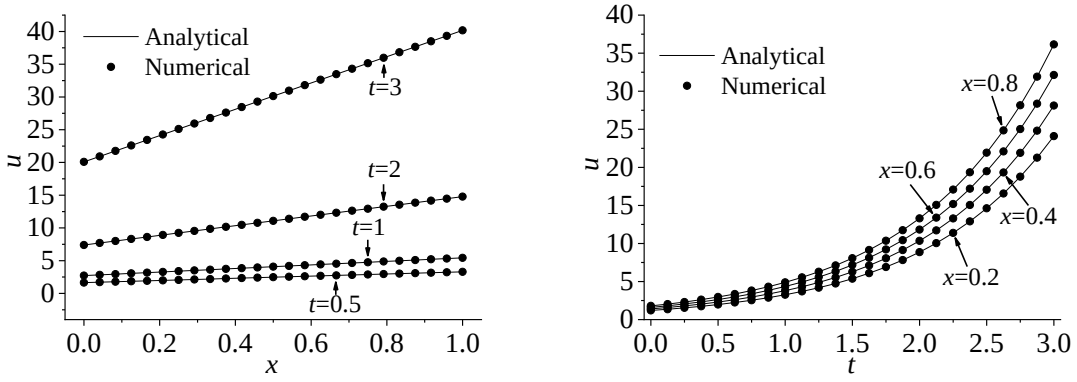
Table3 presentsthe absolute errors considering the influence of *NCP* for the third case study for x = [0.2 0.4 0.6 0.8] and t is equal to the unity.

Table 3: Absolute error computed for the third case study considering different values for NCP ([2 3 4 5]), x ([0.2 0.4 0.6 0.8]) and t is equal to unity.

NCP	***x*=0.2**	***x*=0.4**	***x*=0.6**	***x*=0.8**	**PT (s)**
2	8.9899×10^{-6}	7.8981×10^{-6}	7.0043×10^{-6}	3.4547×10^{-6}	0.0233
3	1.4367×10^{-7}	2.0676×10^{-7}	6.1210×10^{-7}	4.5345×10^{-7}	0.0678
4	4.5601×10^{-8}	2.0454×10^{-8}	1.0676×10^{-7}	4.5066×10^{-8}	0.5678
5	2.0451×10^{-9}	3.4055×10^{-9}	7.0890×10^{-9}	1.0223×10^{-9}	0.8987

As observed for the first two applications, the increase in the value of the number of collocation points implies in an increase of an ordinary differential system to be integrated. As a consequence, a more accurate solution is obtained. As seen in previous case studies, the processing time is proportional to the value of *NCP*, i.e., greater values for this parameter imply longer processing times. Regarding the work of Lakestani and Dehghan (2009) [13], the obtained results using the OCM are in agreement with *NCP* equal to 5, as the absolute error is of the order of, approximately, 10^{-9} in t equal to unity.

Figures 3a and 3b presents the dependent profiles considering *NCP* equal to 5, t = [0.5 1 2 3] and x = [0.2 0.4 0.6 0.8]. In this figure, we can observe a good agreement between analytical and numerical solutions, demonstrating the quality of the proposed methodology.



(a) $u\times x$. (b) $u\times t$.

Figure 3: Analytical versus numerical profiles for the third case study.

5. CONCLUSIONS

In this contribution, the Orthogonal Collocation Method associated to the Runge-Kutta-Fehlberg Method is considered as a numerical strategy to solve linear Fokker-Planck equations. The proposed methodology was applied to three case studies that present analytical solution. The obtained results demonstrate a good performance of the proposed methodology when the estimated error is evaluated. It should be noted that the final system to be integrated depends on the number of collocation points and the number of discretization points required by the solver

used to integrate the initial value ordinary differential equations. Thus, the relation convergence versus the processing time can be optimized to obtain the best configuration between these inputs in future applications.

Further research will be focused on the inclusion of reliability and robustness to solve inverse problems considering the Fokker-Planck equation, as well as the study considering the fractional context.

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