Using Chebyshev Polynomials in Solving Diffusion Equations

Ghuson S Abed

University of Information Technology and Communications, Iraq

E-mail: Ghsonabed.2019@uoitc.edu.iq

Abstract. In this work, we modified Chebyshev polynomials of the first kind to match the characteristics of a second order differential equation that is a result of a separation of the variable technique used to solve a partial differential diffusion equation. The resultant polynomials solution in one spatial dimension is found and the corresponding changing parameters for the first order differential equation in time are extracted accordingly. The method is tested for applicability, stability, and convergence.

1. Introduction

Differential Equations (DEs) are widely used as models for variables behavior in many phenomena in different fields of science. While setting DE to the model certain phenomenon can be achieved if all the variables, parameters, and relations are known, the solution of this DE is another story. An only a small fraction of different types of DEs can be solved analytically and exactly, while most of them have no known analytical exact solution. Partial Differential Equations (PDEs) represent a special type of DEs, where two or more independent variables exist, and they have special importance in the fields of engineering and physics. PDEs have no analytical exact solution in most cases; so many techniques are used to find an approximate solution instead. These techniques can be classified into two major types: numerical solution and series solution. Each technique has its advantages and disadvantages. The numerical solution, mainly by using a finite difference technique, has the advantages of both simplicity and wide applicability if convergence criteria are followed. The disadvantage of the numerical solution is the non function results representation, the result is only values of the variables at the limited number of nodes specified by the solution. The series solution has the advantage of representing the solution as a sum of analytical functions applied at all the space of the problem, but to achieve this task more complicated steps and different approaches are needed for different DEs. One of the most powerful methods used to solve PDEs is using Orthogonal Polynomials (OPs) together with the separation of variables technique [17, 18, 3, 19, 9]. Different other techniques also used such as the Fokas method [6, 1, 2]. There are different types of OPs, most of them were used for solving DEs. Among them, Fourier series are widely used, due to their characters that their second derivatives are a constant multiple of their values that match, widely used, second order DEs [26, 25, 15, 12]. But when the Fourier series is not compatible with the problem symmetry and/or boundary values, then other OPs can be used, where they can be matched to the problem boundary conditions [7,4,21,24,16,5], or they can be matched to the problem symmetry [20] and develop a correct solution. Chebyshev Polynomials CPs are OPs, which have many interesting properties [22, 29, 11]. CPs are widely used in fitting due to their high efficiency in reducing the error of interpolation [27], and for that, they are used to find the particular solution of different types of DEs [23]. CPs are also used in solving different types of DEs [8,13,10,28].
In this work we used CPs of the first kind [22] and the separation of variables technique, to solve the diffusion equation. CPs is modified to match the diffusion equation characteristics and boundary conditions. The strategy is tested for convergence and stability, and the results are compared with that of well-known method of using the Fourier series and separation of variables that compatible with the chosen examples.

2. Problem definitions:

2.1 Diffusion equation
The diffusion equation represents a time varying, the spatial balance of specific particles that are generated, absorbed, and leaked out/in due to non field diffusion [14]. Diffusion equation in a homogeneous medium can be written as:

\[
\frac{1}{v} \frac{\partial \theta(r, t)}{\partial t} - D \nabla^2 \theta(r, t) = s(r, t) - \sum a \cdot \theta(r, t)
\]

(1)

Where:
First term: Particles flux rate of change with time
Second term: Particles leakage rate
Third term: Particles generation rate
Fourth term: particles absorbing rate

2.2 Orthogonal series
Any continuous function can be expanded in an infinite series as:

\[
f(x) = \sum_{i=0}^{\infty} a_i \cdot s_i(x)
\]

(2)

An orthogonal series is a special type, with the property:

\[
\int_{x1}^{x2} s_i(x) \times s_j(x) \times w(x) = \begin{cases} 
0 & i \neq j \\
\text{constant} & i = j
\end{cases}
\]

(3)

Chebyshev Polynomials \( \sum_{i=0}^{\infty} a_i \cdot T_i(x) \), and trigonometric polynomials \( \sum_{i=0}^{\infty} a_i \cdot \cos(i\pi x) \), are examples of orthogonal polynomials.

2.3 Problem setting and examples
Normalizing the problem, eq. (1), by setting: \( v = 1 \), \( D = 1 \), \( \sum a = 1 \) and let: \( s(x, t) = K \cdot \sum a \cdot \theta(x, t) \), \( K: \text{constant} \). Equation (1) in one spatial dimension will be

\[
\frac{\partial \theta(x, t)}{\partial t} - \frac{\partial^2 \theta(x, t)}{\partial x^2} = (k - 1) \cdot \theta(x, t)
\]

(4)

The method will be tested for two examples:
Example A, have a spatial symmetrical initial condition:
\[
\theta(x, 0) = 4x(1 - x); \quad \theta(0, t) = 0; \quad \theta(1, t) = 0
\]

(5A)

Example B, asymmetrical initial condition:
\[ \emptyset(x, 0) = x(1 - x)(2 - x)(3 - x); \emptyset(0, t) = 0; \emptyset(1, t) = 0 \]  

(5B)

3. Solution using Fourier analysis and Separation of Variables (SFASV).

Let
\[ \emptyset(x, t) = \emptyset(x). \emptyset(t) \]  

(6)

Equation (4) will be:
\[
\begin{align*}
\emptyset(x) \frac{d\emptyset(t)}{dt} - \emptyset(t) \frac{d^2\emptyset(x)}{dx^2} &= (k - 1) \emptyset(x). \emptyset(t) \\
\frac{1}{\emptyset(t)} \frac{d\emptyset(t)}{dt} - \frac{1}{\emptyset(x)} \frac{d^2\emptyset(x)}{dx^2} &= (k - 1)
\end{align*}
\]

(7)

(8)

Equation (8) can be split to two equations:
\[
\begin{align*}
\frac{1}{\emptyset(t)} \frac{d\emptyset(t)}{dt} &= a_1 \\
\frac{1}{\emptyset(x)} \frac{d^2\emptyset(x)}{dx^2} &= -(b_1)^2
\end{align*}
\]

(9)

(10)

Where their solutions are:
\[
\begin{align*}
\emptyset(t) &= A_2. e^{a_1.t} \\
\emptyset(x) &= B_1. cos(b_1.x) + B_2. sin(b_1.x)
\end{align*}
\]

(11)

(12)

The general solution will be
\[ \emptyset(x, t) = [C_1. cos(b_1.x) + C_2. sin(b_1.x)]. e^{a_1.t} \]  

(13)

From the boundary condition \( \emptyset(0, t) = 0 \), one can find that \( C_1 = 0 \).

From the boundary condition \( \emptyset(1, t) = 0 \), one can find that: \( b_1 = n. \pi, \ n = 1(1)\infty \)

Note that \( a_1 + (b_1)^2 = (k - 1) \), hence \( a_1 = (k - 1) - (n\pi)^2 \)

Then the solution will be:
\[
\emptyset(x, t) = \sum_{n=1(1)\infty} C_n. sin(n\pi.x). e^{((k-1)-(n\pi)^2)t}
\]

(14)

And from the initial condition: \( \emptyset(x, 0) = 4x(1 - x) \)
\[ \emptyset(x, 0) = \sum_{n=1(1)\infty} C_n. sin(n\pi.x) \]  

(15)

This will give:
\[
C_n = 2 \int_{0}^{1} \emptyset(x, 0). sin(n\pi.x) \ . dx
\]

(16)
Moreover, for the given examples:

\[ C_n = 2 \int_0^1 4x(1 - x).\sin(n\pi x) \, dx \]  
(17A)

\[ C_n = 2 \int_0^1 x(1 - x)(2 - x)(3 - x).\sin(n\pi x) \, dx \]  
(17B)

\[ C_n = \frac{32}{(n\pi)^3}, \quad n = 1(2)^\infty, \text{odd} \]  
(18A)

\[ C_n = 0, \quad n = \text{even} \]  

\[ C_n = \frac{48}{(n\pi)^3}, \quad n = 2(2)^\infty, \text{even} \]  
(18B)

\[ C_n = \left[ \frac{40}{(n\pi)^3} - \frac{96}{(n\pi)^5} \right], \quad n = 1(2)^\infty, \text{odd} \]  

Then (14) will be:

\[ \emptyset(x, t) = \sum_{n=1(2)^\infty} \left[ \frac{32}{(n\pi)^3} \right] \sin(n\pi x) \cdot \exp\left(\left((k - 1) - (n\pi)^2\right) \cdot t\right) \]  
(19A)

\[ \emptyset(x, t) = \sum_{n=2(2)^\infty} \left[ \frac{48}{(n\pi)^3} \right] \sin(n\pi x) \cdot \exp\left(\left((k - 1) - (n\pi)^2\right) \cdot t\right) \]  

\[ + \sum_{n=1(2)^\infty} \left[ \frac{40}{(n\pi)^3} - \frac{96}{(n\pi)^5} \right] \sin(n\pi x) \cdot \exp\left(\left((k - 1) - (n\pi)^2\right) \cdot t\right) \]  
(19B)

4. Solution using Chebyshev Polynomials and Separation of Variables (SCPSV).

Chebyshev polynomials of the first kind have the following recurrence relations [22].

\[ T_1(x) = 1, \quad T_2(x) = x, \quad T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \]

They are listed with their second derivatives up to i=9 in Table1.

| i   | \(T_i(x)\) | \(T_i''(x)\) |
|-----|-------------|---------------|
| 1   | 1           | 0             |
| 2   | x           | 0             |
| 3   | \(2x^2-1\)  | 4             |
| 4   | \(4x^3-3x\) | 24x           |
| 5   | \(8x^4-8x^2+1\) | 96x^2-16  |
| 6   | \(16x^5-20x^3+5x\) | 320x^3-120x |
| 7   | \(32x^6-48x^4+18x^2-1\) | 960x^4-576x^2+36 |
| 8   | \(64x^7-112x^5+56x^3-7x\) | 2688x^5-2240x^3+336x |
| 9   | \(128x^8-256x^6+160x^4-32x^2+1\) | 7168x^6-7680x^4+1920x^2-64 |

We have equation (4): \(\frac{\partial \emptyset(x,t)}{\partial t} - \frac{\partial^2 \emptyset(x,t)}{\partial x^2} = (k - 1) \emptyset(x,t)\), and the boundaries are: \(x = [0,1]\), and \(t_{\text{initial}} = 0\).
Note that for the problem \( \{x=[0,1], t=[0,\infty)\} \), while Chebyshev polynomials are defined in the interval \( \{y=(-1,1)\} \). Therefore, axis transformation is required. Let: \( x = \frac{y+1}{2} \), \( y = 2x - 1 \). Then (4, 9, and 10) will be:

\[
\frac{\partial \phi(y, t)}{\partial t} - 4 \frac{\partial^2 \phi(y, t)}{\partial y^2} = (k - 1) \phi(y, t) \tag{4.1}
\]

\[
\frac{1}{\partial t} d\phi(t) = a_1 \tag{4.2}
\]

\[
\frac{d^2 \phi(y)}{dy^2} = -\left(\frac{b_1}{2}\right)^2 \phi(y) \tag{4.3}
\]

The boundaries are \( y = [-1,1] \), and \( t_{\text{initial}}=0 \), and where for example (A):

\( \phi(y, 0) = (1 - y^2) ; \phi(-1, t) = 0 ; \phi(1, t) = 0 \)

And for example (B):\( \phi(y, 0) = \left(\frac{15-8y-14y^2+8y^3-y^4}{16}\right) \); \( \phi(-1, t) = 0 ; \phi(1, t) = 0 \)

Let the solution of (10.1) is:

\[
\phi y(y) = \sum_{i=1}^{\infty} c_i \phi y_i(y) \tag{20}
\]

\[
\phi y_i(y) = (T_i(y) - T_{i+2}(y)) + EP \tag{21}
\]

And the total solution is:

\[
\phi(y, t) = \sum_{i=1}^{\infty} c_i \phi y_i(y) \cdot \exp(a_{1i} \cdot t) \tag{22}
\]

\[ a_{1i} = (k - 1) - (i\pi)^2 \]

Where Equation Polynomial is an extension to \((T_i(y) - T_{i+2}(y))\) that will make the second derivative of \( \phi y_i(y) \) a constant, \(-\left(\frac{b_1}{2}\right)^2\), multiple of \( \phi y_i(y) \) itself, and matching the characteristics of (10.1). To find the \( EP(\text{extended polynomial}) \), multiply the second term in the function \((T_i(y) - T_{i+2}(y))\) by the value of \(-\left(\frac{b_1}{2}\right)^2\), and add it to the second derivative, and add its double integral to the function, and so on. Some \( \phi y_i(y) \), their second derivatives, and the corresponding \(-\left(\frac{b_1}{2}\right)^2\) values are shown in Table2.

**Table2:** Some \( \phi y_i(y) \), their second derivatives, and \(-\left(\frac{b_1}{2}\right)^2\) values.

| \( i \) | \( T_i(y) \) | \( \phi y_i(y) = T_i(y) - T_{i+2}(y) + EP \) | \( \frac{d^2 \phi y(y)}{dy^2} \) | \(-\left(\frac{b_1}{2}\right)^2\) |
|---|---|---|---|---|
| 1 | \(-y^{10}/56700+y^{9}/1260+y^{8}/45+y^{4}/3-2y^2+2\) | \(-y^{8}/630+2y^{6}/45-2y^{4}/3+4y^{2}-4\) | -2 |
| 2 | \(-y^{11}/3850+y^{9}/70+y^{6}/35+y^{5}/5-2y^{3}+4y\) | \(-y^{7}/35+36y^{7}/35-36y^{6}/5+24y^{5}/24y\) | -6 |
| 3 | \(3125y^{14}/13621608-625y^{13}/149688+125y^{10}/2268-125y^{8}/252+25y^{7}/9-y^{5}/3-8y^{4}/3+4y^{2}-2\) | \(3125y^{12}/74844-625y^{11}/1134+625y^{9}/126-250y^{8}/9+250y^{7}/3-4y^{5}/96y^{4}+20\) | -10 |
Note that:

\[(b_i)^2(s)=4s^2+4, \quad s=\text{odd} \quad (23)\]
\[(b_i)^2(s)=4s^2+8, \quad s=\text{even} \quad (24)\]

\[\varnothing y_i(y) = \sum_{j=1,3,5}^{\infty} (-1)^{s-1} \frac{s-1}{2} \left( \frac{b_i^2}{4} \right)^{\frac{j-1}{2}} \frac{y^{-1}}{(j-1)!} \quad (25)\]

\[\varnothing y_i(y) = \sum_{j=2,4,6}^{\infty} (-1)^{s+2} \frac{s+2}{2} \left( \frac{b_i^2}{4} \right)^{\frac{j-1}{2}} \frac{y^{-1}}{(j-1)!} \quad (26)\]

Note that the solution in (22), SCPSV, is a floating solution with respect to the boundary conditions. This represents an advantage, that it can be used for any boundary conditions while SFASV is limited to zero boundary conditions. To match the solution to the problem boundary conditions, the stated boundary conditions and that obtained from the floating solution are matched by a quadratic function in the spatial dimension, since it is the order of \(\varnothing y_1(y)\). This show reasonable stability and convergence.

5. Results and discussion:
The (SFASV) is found according to (19) for the two examples. The solutions are modeled using Matlab, and it is found that the results are stable for \(N=7\) (n truncated at 7). The (SCPSV) are also found according to (22) using Matlab, for different values of \(N\) (series truncation value of i), where \(\varnothing y_i(y)\) are found according to (25 &26) and where \(j\) truncated at different \((M_i)\) values (\(M=1, 2, &3\) are used), and where for \(M>3\) there are no effective changes in the results. \((b_i)\) values are found by (23&24) and \(C_i\) values are found by a least-square fitting of \(\varnothing y_i(y)\) to the initial condition, according to (20).The total transient solutions for \((k=20, \ t_{final}=0.1)\) by SFASV with \(N=7\) and by SCPSV with \(N=25, M=3\) are shown in Fig. (1) for example A and in Fig. (2) for Example B. While total transient solution figures show no differences between the two methods, one can use better descriptive comparisons. Fig. (3&4) shows the solutions by SCPSV for different \(N&M\) values compared to the solution by SFASV with \(N=7\), for examples A & B respectively. Fig. (5) shows an average of the absolute difference of the whole solutions between SFASV with \(N=7\) and SCPSV for different \(N \& M\) values, for example, B. Example A shows the same behavior. Figures (3, 4 &5) show clearly the SCPSV stability and convergence with \(N \& M\) values.
Fig (1): Comparison between SFASV & SCPSV for examples A

Fig (2): Comparison between SFASV & SCPSV for examples B

N=5, M=1

N=5, M=1
Fig (3): The solution at $t_{ini} = 0.1$, by SCPSV for different $N$ & $M$ values compared to SFASV solution with $N=7$, for Example B.

Fig (4): The solution at $t_{ini} =0.1$, by SCPSV for different $N$ & $M$ values compared to SFASV solution with $N=7$, for Example A

Fig(5): Average of the absolute difference of the whole solutions between SFASV with $N=7$ and SCASV, for different $N$ & $M$ values, for example B.
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