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Polymer nanofibers deposited via coaxial electrospinning: A model for core-shell structured through solutions to Lane-Emden equation

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ABSTRACT

In this paper, a model to core-shell structured polymer nanofibers deposited via coaxial electrospinning is presented. Investigations are based on a modified Jacobi-Gauss collocation spectral method, proposed along with the Boubaker Polynomials Expansion Scheme *BPES*, for providing solution to a nonlinear Lane-Emden type equation. The spatial approximation has been based on shifted Jacobi polynomials $P_{T,N}^{(\alpha,\beta)}(x)$ with $\alpha,\beta \in (-1,\infty), T>0$ and *n* was the polynomial degree. The Boubaker Polynomials Expansion Scheme *BPES* main feature, concerning the embedded boundary conditions, have been outlined. The modified Jacobi-Gauss points are used as collocation nodes. Numerical examples are included to demonstrate the validity and applicability of the technique and a comparison is made with existing results. It has been revealed that both methods are easy to implement and yields very accurate results.

KEYWORDS

Core-shell structured nanofibers;
Polymers;
Lane-emden type equation;
Second-order initial value problems;
BPES;
Collocation method;
Jacobi-gauss quadrature;
Shifted Jacobi polynomials.

INTRODUCTION

Polymer nanofibers have gained much attention due to their great potential applications, such as filtration, catalysis, scaffolds for tissue engineering, protective clothing, sensors, electrodes electronics applications, reinforcement and biomedical use[1-6]. Particularly, polymeric nanofibers with core-shell structure have been attractive in the past decades[4,5]. Co-axial electrospinning, which has emerged as a method of choice due to the simplicity of the technology and its cost effectiveness, provides an effective and versatile way to fabricate such nanofibers[6-8]. This technique uses a high electric field to extract a liquid jet of polymer solution from the bot core and shell reservoirs. The yielded jet experiences stretching and bending effects due to charge repulsion and, in the process, can reach very small radii. Co-axial electrospinning can not only be used to spin the unspinnable polymers (Polyaramid, nylon and poly-aniline) into ultrafine fibers, but also ensures keeping functionalizing agents like antibacterial and biomolecules agents inside nanofibers[9-11].

In this paper, a mathematical model to coaxial electrospinning dynamics, in a particular setup, is presented. The model is based on solutions to the related Lane-Emden equation on semi-infinite domains:

$$u''(x)+\frac{a}{x}u'(x)=g(x,u(x)); \quad 0<x<\infty \tag{1}$$

Lane-Emden type equations model many phenomena in mathematical physics and nano-applications. They were first published by Lane in 1870[12], and further explored in detail by Emden[13]. In the last decades, Lane-Emden has been used to model several phenomena such as the theory of stellar structure, quantum mechanics, astrophysics and the theory of thermionic currents in the neighbourhood of a hot body in thermal equilibrium and the thermal behaviourof an isothermal gaseous sphere[14-18]. Even if Lane-Emden problem was numerically challenging because of the singularity behavior at the origin, several methods have been used in order to solve it in semi-infinite domains. Boyd[19] used domain truncation method replacing the semi-inûnite domain with [0,K] interval by choosing K, sufûciently large, while Shen[20] used spectral-Galerkin approximations based on Laguerre functions to perform analytical solutions and demonstrated that they were stable and convergent with spectral accuracy in the Sobolev spaces. Maday *et al.*[21] proposed a Laguerre type spectral method, Siyyam[22] applied two numerical methods using the Laguerre Tau method, and Guo[23] reformulated the original Lane-Emden problem to a singular problem in a bounded domain by variable transformation using the Jacobi polynomials.

This paper is organized as follows: In Section 2 we present an illustrated formulation of the problem, then, in Section 3, we give an overview of the modified Jacobi-Gauss collocation spectral method along with its applications, and in Sections 4, we present the fundaments and the application of the Boubaker Polynomials Expansion Scheme BPES. In Section 5, results are plotted and discussed along wirh comparison with some existing solutions. A conclusion is given in Section 6.

PROBLEM FORMULATION

As per Spivak *et al.*[24,25], mass balance, linear moentum balance and electric charge balance equations describe polymer fibers electrospinning process:

$$\nabla.\vec{u}=0 \tag{2}$$

$$\rho(\vec{u}.\nabla)\vec{u}=\nabla F^m+\nabla F^e \tag{3}$$

$$\nabla.\vec{J}=0 \tag{4}$$

where $\vec{u}$ is the axial velocity, $\vec{J}$ is the electrical current density, ρ is material density, F^m and F^e are terms which represent viscous and electric forces, respectively.

Under the assuptions of a steady state jet and a neglectible thermal effort, the electrically generated force is dominant, the monodimentional momentum equation is hence:

$$u\frac{\partial u(x)}{\partial x}=\frac{2\sigma(x)E(x)}{\rho r} \tag{5}$$

where u is the modulus of the axial velocity, r is the radius of the jet at axial coordinate x (Figure 1), $\sigma(x)$ is the surface charge density, and E is the exogenous electric field in the axial direction.

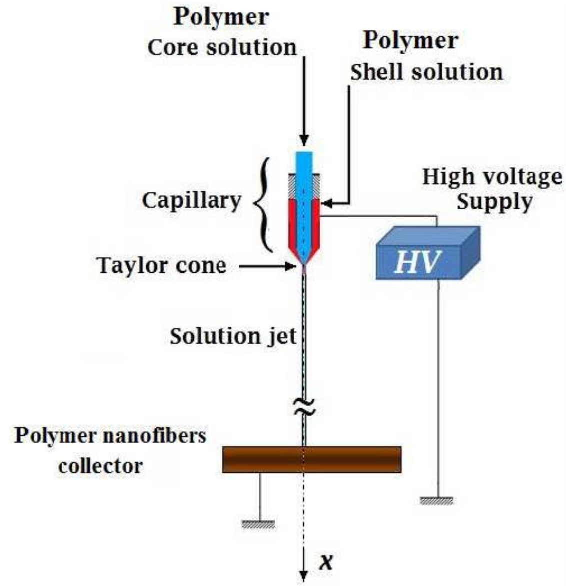

Figure 1 : Scheme of the studied setup

By introducing the charge balance equation:

$$2r\sigma(x)u(x)+r^2kE(x)=I \tag{6}$$

where I is the electrical current intensity and k is a constant which depend only on temperature in the case of an incompressible polymer, it gives:

$$u\frac{\partial u(x)}{\partial x}=\frac{E(x)(I-r^2kE(x))}{\rho r^2 u} \tag{7}$$

Then, by introducing the variable:

$$y=-6Ln(u) \tag{8}$$

it gives:

$$\frac{\partial y}{\partial x}=-\frac{6E(x)(I-r^2kE(x))}{\rho r^2}e^{y/2} \tag{9}$$

By differentiating the last equation, along with assuming weak r-dependence of the variable x, we have:

$$\frac{\partial^2 y}{\partial x^2}-\left(-\frac{6\frac{dE(x)}{dx}}{\rho r^2}Ie^{y/2}+\frac{\frac{12dE(x)}{dx}}{\rho^2}E(x)e^{y/2}-\frac{3E(x)(I-r^2kE(x))}{\rho r^2}e^{y/2}\frac{\partial y}{\partial x}\right)=0 \tag{10}$$

and by choosing the exogenous electric field profile so that:

$$\begin{cases}\frac{3E(x)(I-r^2kE(x))}{\rho r^2}=\frac{2}{x}e^{-3Ln(u)/2}\\ -\frac{6\frac{dE(x)}{dx}}{\rho r^2}Ie^{y/2}+\frac{\frac{12dE(x)}{dx}}{\rho^2}E(x)e^{y/2}=-6Ln(u)(-6-4Ln(-6Ln(u))e^{-3Ln(u)/2}\end{cases} \tag{11}$$

it gives, by annexing boundary conditions:

$$\begin{cases}\frac{\partial^2 y}{\partial x^2}+\frac{2}{x}\frac{\partial y}{\partial x}-6y(x)=4y(x)Ln(y(x))\\ y(0)=1\ \&\\ y'(0)=0\end{cases} \tag{12}$$

MODIFIED JACOBI-GAUSS COLLOCATION MJGC METHOD

Let $\alpha>-1,\beta>-1$ and $P_k^{(\alpha,\beta)}$ be the standard Jacobi polynomial of degree k. We have :

$$\begin{cases}P_k^{(\alpha,\beta)}(-x)=(-1)^k P_k^{(\alpha,\beta)}(x), P_k^{(\alpha,\beta)}(-1)=\frac{(-1)^k\Gamma(k+\beta+1)}{k!\Gamma(\beta+1)}\\ P_k^{(\alpha,\beta)}(1)=\frac{\Gamma(k+\beta+1)}{k!\Gamma(\beta+1)}\end{cases} \tag{13}$$

Then, let $T>0$, then the shifted Jacobi polynomial of degree k on the interval $(0,T)$ is defined by :

$$P_{T,k}^{(\alpha,\beta)}(x)=P_k^{(\alpha,\beta)}(\frac{2x}{T}-1) \tag{14}$$

Consequently, we have :

$$\begin{cases}P_{T,k}^{(\alpha,\beta)}(0)=(-1)^k\frac{\Gamma(k+\beta+1)}{k!\Gamma(\beta+1)}\\ D^q P_{T,k}^{(\alpha,\beta)}(0)=\frac{(-1)^{k-q}\Gamma(k+\beta+1)(k+\alpha+\beta+1)q}{T^q\Gamma(k-q+1)\Gamma(q+\beta+1)}\end{cases} \tag{15}$$

For $\alpha=\beta$ one recovers the shifted ultraspherical polynomials (symmetric shifted Jacobi polynomials) and for $\alpha=\beta=\mp\frac{1}{2},\alpha=\beta=0$ the shifted Chebyshev of the first and second kinds and shifted Legendre polynomials respectively; and for the nonsymmetric shifted Jacobi polynomials, the two important special cases $\alpha=-\beta=\pm\frac{1}{2}$

(shifted Chebyshev polynomials of the third and fourth kinds) are also recovered.

Jacobi-Gauss interpolation starts by denoting $x_{N,j}^{(\alpha,\beta)} 0 \le j \le N$ the nodes of the standard Jacobi-Gauss interpolation. The corresponding Christoffel numbers are $\varpi_{N,j}^{(\alpha,\beta)} 0 \le j \le N$. The nodes of the shifted Jacobi-Gauss interpolation on the interval (0, *T*) are the zeros of $P_{T,N+1}^{(\alpha,\beta)}(x)$, denoted by $x_{T,N,j}^{(\alpha,\beta)} = (T/2)^{\alpha+\beta+1}\varpi_{N,j}^{(\alpha,\beta)}$. The corresponding Christoffel numbers are $\varpi_{T,N,j}^{(\alpha,\beta)} = (T/2)^{\alpha+\beta+1}\varpi_{N,j}^{(\alpha,\beta)}$. Let $S_N(0,T)$ be the set of polynomials of degree at most *N*. Thanks to the property of the standard Jacobi-Gauss quadrature, it follows that for any $\Lambda \in S_{2N+1}(0,T)$:

$$\int_0^T (T-x)^\alpha x^\beta \Lambda(x)dx = \left(\frac{\tau}{2}\right)^{\alpha+\beta+1} \int_{-1}^1 (1-x)^\alpha (1+x)^\beta x^\beta \Lambda\left(\left(\frac{T}{2}\right) x_{N,j}^{(\alpha,\beta)} + 1\right) dx$$
$$= \left(\frac{\tau}{2}\right)^{\alpha+\beta+1} \sum_{j=0}^{N} \varpi_{T,N,j}^{(\alpha,\beta)} \Lambda\left(x_{T,N,j}^{(\alpha,\beta)}\right) \quad (16)$$

where $x_{T,N,j}^{(\alpha,\beta)}$ and $\varpi_{T,N,j}^{(\alpha,\beta)}$ are the nodes and the corresponding weights of the shifted Jacobi-Gauss-quadrature formula on the interval (0,*T*), respectively.

For solving (12), we first set:

$$S_N(0,T) = \operatorname{span}\left\{P_{T,0}^{(\alpha,\beta)}(x), P_{T,1}^{(\alpha,\beta)}(x), \cdots, P_{T,N}^{(\alpha,\beta)}(x)\right\} \quad (17)$$

Thus, for any $u \in S_N(0,T)$, the norms $\|u\|_{w_T^{(\alpha,\beta)},N}$ and $\|u\|_{w_T^{(\alpha,\beta)}}$ coincide.

Associating with this quadrature rule, we denote by $I_N^{P_T^{(\alpha,\beta)}}$ the shifted Jacobi-Gauss interpolation:

$$I_N^{P_T^{(\alpha,\beta)}} u\left(x_{T,N,j}^{(\alpha,\beta)}\right) = u\left(x_{T,N,j}^{(\alpha,\beta)}\right); \quad 0 \le k \le N \quad (18)$$

The shifted Jacobi-Gauss collocation method for solving (xxx) is to seek $z_N(x) \in S_N(0,T)$, such that:

$$z_N(x) = \sum_{j=0}^{N} a_j P_{T,j}^{(\alpha,\beta)}(x), \quad a = (a_0, a_1, \cdots a_N) \quad (19)$$

Let:

$$z_N(x) = \sum_{j=0}^{N} a_j P_{T,j}^{(\alpha,\beta)}(x), \quad a = (a_0, a_1, \cdots a_N) \quad (20)$$

We first approximate z(x), z′(x) and z″(x), as Eq. (19). By substituting these approximation in Eq. (19), we get:

$$\frac{1}{4}\sum_{j=0}^{N} a_j (j+\alpha+\beta+1) P_{T,j-2}^{(\alpha+2,\beta+2)}(x_{T,N,k}^{(\alpha,\beta)}) +$$
$$\frac{1}{2}\sum_{j=0}^{N} a_j (j+\alpha+\beta+1) P_{T,j-1}^{(\alpha+1,\beta+1)}(x_{T,N,k}^{(\alpha,\beta)})^2$$
$$+ \frac{2}{x_{T,N,k}^{(\alpha,\beta)}} \frac{1}{2}\sum_{j=0}^{N} a_j (j+\alpha+\beta+1) P_{T,j-1}^{(\alpha+1,\beta+1)}(x_{T,N,k}^{(\alpha,\beta)}) \quad (21)$$
$$+ 4\sum_{j=0}^{N} a_j P_{T,j}^{(\alpha,\beta)}(x_{T,N,k}^{(\alpha,\beta)}) + 6$$

Next, after using (13) and (15) at $q = 1$, we have:

$$\begin{cases} \sum_{j=0}^{N} (-1)^j \dfrac{\Gamma(j+\beta+1)}{j!\Gamma(\beta+1)} a_j = 0 \\ \sum_{j=0}^{N} (-1)^{j-1} \dfrac{\Gamma(j+\beta+1)(j+\alpha+\beta+1)}{T(j-1)!\Gamma(\beta+2)} a_j = 0 \end{cases} \quad (22)$$

Finally, from (19), (21) and (22), we get (N + 1) nonlinear algebraic equations which can be solved for the unknown coefficients a_j by using any standard iteration technique, like Newton's iteration method. Consequently, $z_N(x)$ given in Eq. (20) can be evaluated, and then the approximate solution of (12) can be obtained.

The boubaker polynomials expansion scheme BPES

The Boubaker Polynomials Expansion Scheme BPES[26-35] is a resolution protocol which as been successfully applied to several applied-physics and mathematics problems. The BPES protocol ensures the validity of the related boundary conditions regardless main equation features. The BPES is mainly based on Boubaker polynomials first derivatives properties:

$$\begin{cases} \left.\sum_{q=1}^{N} B_{4q}(x)\right|_{x=0} = -2N \ne 0; \\ \left.\sum_{q=1}^{N} B_{4q}(x)\right|_{x=r_q} = 0; \end{cases} \quad (23)$$

and:

$$\begin{cases} \sum_{q=1}^{N} \left.\dfrac{dB_{4q}(x)}{dx}\right|_{x=0} = 0 \\ \sum_{q=1}^{N} \left.\dfrac{dB_{4q}(x)}{dx}\right|_{x=r_q} = \sum_{q=1}^{N} H_q \\ \text{with : } H_n = B'_{4n}(r_n) = \left(\dfrac{4r_n[2-r_n^2]\times\sum_{q=1}^{n} B_{4q}^2(r_n)}{B_{4(n+1)}(r_n)} + 4r_n^3 \right) \end{cases} \quad (24)$$

Several solution have been proposed through the BPES in many fields such as numerical analysis[26], material characterization[27], theoretical physics[28], mathematical algorithms[29], heat transfer[31,32] and homo dynamics[33-35].

The Boubaker Polynomials Expansion Scheme BPES is applied to the system (12) through setting the expression:

$$u(x) = \frac{1}{2N_0}\sum_{k=1}^{N_0} \lambda_k \times B_{4k}(xr_k) \quad (25)$$

where B_{4k} are the 4k-order Boubaker polynomials, x $\in [0,1]$ is the normalized variable, r_k are B_{4k} minimal positive roots, N_0 is a prefixed integer and $\lambda_k|_{k=1..N_0}$ are unknown pondering real coefficients.

Thanks to the properties expressed by Equations (23) and (24), boundary condition are trivially verified in advance to resolution process. The system (1) is hence reduced to:

$$\begin{cases} \dfrac{1}{2N_0}\sum_{k=1}^{N_0} \lambda_k \times \dfrac{d^2B_{4k}(xr_k)}{dx^2} + \\ \dfrac{1}{xN_0}\sum_{k=1}^{N_0} \lambda_k \times \dfrac{dB_{4k}(xr_k)}{dx} - \dfrac{3}{N_0}\sum_{k=1}^{N_0} \lambda_k \times B_{4k}(xr_k) = \\ \dfrac{2}{N_0}\sum_{k=1}^{N_0} \lambda_k \times B_{4k}(xr_k) Ln(\dfrac{1}{N_0}\sum_{k=1}^{N_0} \lambda_k \times B_{4k}(xr_k)) \end{cases} \quad (26)$$

The BPES solution is obtained by determining the non-null set of coefficients $\tilde{\lambda}_k|_{k=1..N_0}$ that minimizes the absolute difference Δ_{N_0}:

$$\begin{cases} \Delta_{N_0} = \left| \left(\dfrac{1}{2N_0}\sum_{k=1}^{N_0} \tilde{\lambda}_k \times \Lambda_k \right) - \left(\dfrac{1}{2N_0}\sum_{k=1}^{N_0} \tilde{\lambda}_k \times \Lambda'_k \right) \right| \\ \text{with :} \\ \Lambda_k = r_k^2 \displaystyle\int_0^1 \dfrac{d^2B_{4k}}{dx^2}(x\times r_k)\,dx \\ \Lambda'_k = -r_k \displaystyle\int_0^1 \left(\begin{array}{l} \dfrac{2}{x}\times\dfrac{dB_{4k}}{dx}(x\times r_k) + \\ \left(6 + 4Ln(\dfrac{1}{N_0}\sum_{k=1}^{N_0} B_{4k}(x\times r_k)\right) B_{4k}(x\times r_k) \end{array} \right) dx \end{cases} \quad (27)$$

The final solution is hence:

$$u(x) = \frac{1}{2N_0}\sum_{k=1}^{N_0} \tilde{\lambda}_k \times B_{4k}(xr_k) \quad (28)$$

RESULTS PLOTS AND DISCUSSION

Plots of the solution obtained by the modified Jacobi-Gauss collocation spectral method are presented in Figure 2, along with BPES solution.

According to the results recorded by Theron *et al.*[36], He *et al.*[37,38], Xu *et al.*[39] and Thompson *et al.*[40], velocity at the beginning of the process is jugulated along a short path then is exponentially accelerated. These features are fully verified in the present results (Figure 2). It seems that the two methods ensure the preset boundary condition expressed in Eq. (12). From a methodological point of view, the BPES resolution process forces the validity of the boundary conditions prime to establishment of the resolution algorithm while the modified Jacobi-Gauss collocation spectral method takes boundary conditions into account at the same level with the main equation.

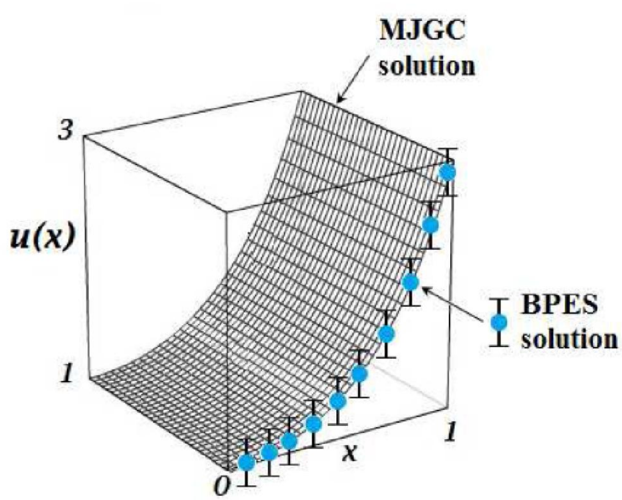

Figure 2 : Solution plots

Figure 2 displays a velocity profile which matches perfectly the conditions evoked by Zhmayev *et al.*[41] and Shin *et al.*[42]. In fact, along an unitary path, jet velocity increases of about 300 percent, which is a favorable condition for fiber formation[41,42].

Additional error analyses yielded a mean relative error below 0.4% (Figure 3).

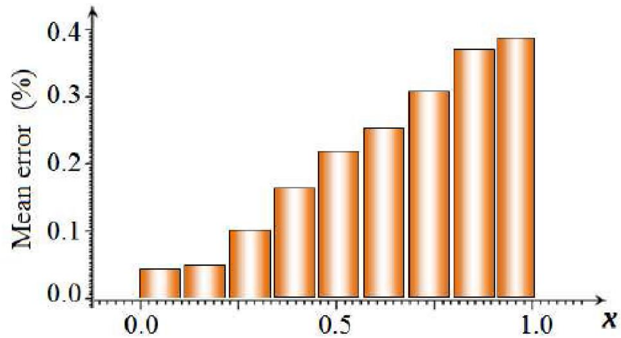

Figure 3 : Mean error analyses

CONCLUSION

The Lane-Emden type equations describe a variety of phenomena in theoretical physics and astrophysics, including polymer fibres electrospinning process dynamics. In this paper we tried to give a founded supply to recerntly proposed related models. Efficient and accurate resolution schemes based on a comparative study of a modified Jacobi-Gauss collocation spectral method and the Boubaker Plynomials Expansion Scheme *BPES* have been used.

Plots and error anaysis illustrations were given to demonstrate the validity and applicability of the method. The results show that the model is not very far from real assumptions and considerations.

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