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Second Order Finite Difference Method for the Thomas-Fermi Equation via Fractional Order of Algebraic and Exponential Mapping Approach

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Abstract

Many problems based on natural sciences need to be solved by the scientists and engineers to serve the humanity. One of the well-known model in atomic universe is condensed into an equation, and called the Thomas-Fermi equation. It is a second order differential equation, which describes charge distributions of heavy, neutral atoms. No exact analytical solution has been found for the equation yet. In fact, strong nonlinearity, singular character and unbounded interval of the problem causes great difficulty to obtain an approximate numerical solution as well. In this paper, the Thomas-Fermi equation is solved using a second order finite difference method along with application of quasi-linearization method. Semi-infinite interval of the problem is converted into [0, 1) using two different coordinate transformations, namely algebraic and exponential mapping. Numerical order of accuracy has been checked using systematic mesh refinements and comparing the calculated initial slope y'(0). Calculated results for initial slope is found in good agreement with the results available in the literature. Lastly, accuracy is improved by the application of the Richardson extrapolation.

Rasyonel Üslü Cebirsel ve Üstel Eşleme Yaklaşımı ile Thomas-Fermi Denklemi için İkinci Derece Doğruluklu Sonlu Farklar Yöntemi

Anahtar Kelimeler
Thomas-Fermi Denklemi; nonlineer ADD; Yarı sonsuz aralık; Sonlu Farklar Metodu; Sanki-lineerleştirme; Aralık eşleme

Öz

Doğa bilimlerine dayalı birçok problemin insanlığa hizmet etmesi için bilim insanları ve mühendisler tarafından çözülmeleri gerekir. Atomik dünyadaki iyi bilinen modellerden biri, bir denklemde yoğunlaşır ve bu denklem Thomas-Fermi denklemi olarak adlandırılır. Thomas-Fermi denklemi ağır, nötr atomların yük dağılımlarını tanımlayan ikinci dereceden bir diferansiyel denklemdir. Denklem için henüz tam bir analitik çözüm bulunamamıştır. Esasen, problemin güçlü nonlineer yapısı, tekil özellik sergilemesi ve sınırsız aralıklı tanım kümesi, yaklaşık sayısal bir çözüm elde etmede de büyük zorluklara yol açmaktadır. Bu makalede, Thomas-Fermi denklemi, sanki-doğrusallaştırma yöntemi ile birlikte ikinci dereceden doğruluklu bir sonlu farklar yöntemi kullanılarak çözülmüştür. Problemin yarı sonsuz aralığı, cebirsel ve üstel eşleme olarak adlandırılan iki farklı koordinat dönüşümü kullanılarak [0, 1) aralığına dönüştürülmüştür. Sayısal doğruluk mertebesi, sistematik ağ sıkılaştırma tekniği kullanılıp hesaplanan başlangıç eğim y'(0) değerlerinin karşılaştırılması ile kontrol edilmiştir. Başlangıç eğimi için hesaplanan sonuçların, literatürde verilen sonuçlarla iyi bir uyum içinde olduğu gösterilmiştir. Son olarak, Richardson ekstrapolasyonunun uygulanmasıyla çözümün doğruluk mertebesi arttırılmıştır.

1. Giriş

Researchers use mathematics to reveal the mystery of the universe by modelling the physical phenomena mostly in differential forms. Engineering problems as well as scientific ones such as heat transfer, ship hydrodynamics, fluid dynamics, strength of marine structures are mostly described in differential equations. Moreover, they are initial and/or boundary value problems in finite, semi-infinite and infinite intervals. However, exact solution of the investigated differential equation of the modelled system is not always available. Therefore, some approximations and approaches should take place to reach to the solution of the problem, which satisfies the requirements of the case or the investigated system.

The Thomas-Fermi model was first presented by Thomas (1927) to determine the effective electric field inside the heavy atoms with four assumptions to condense the model into an equation. Moreover, Fermi (1928) stated that the model is statistically founded to determine the distribution of electrons in a heavy atom, where he considered electrons as a uniform gas around the nucleus. Therefore, Thomas-Fermi equation describes charge distribution of heavy, neutral atoms. The equation is a second order nonlinear and singular differential equation with semi-infinite interval, which is given as

$$\frac{d^2y}{dx^2} = \frac{y^{\frac{3}{2}}}{\sqrt{x}}, y(0) = 1, y(\infty) = 0 \qquad (1)$$

The Thomas-Fermi equation is considered as one of the most important non-linear equation in mathematical physics and attracted many researchers. Baker (1930) searched an analytical solution around $x = 0$ and obtained a series solution as

$$y(x) = 1 + \alpha x + \frac{4}{3}x^{\frac{3}{2}} + \frac{2}{5}\alpha x^{\frac{5}{2}} + \frac{1}{3}x^3 + \cdots \qquad (2)$$

Where α is the initial slope. Sommerfeld (1932) examined the asymptotic behaviour of the problem and reported that:

$$y(x) \sim \frac{144}{x^3} \text{as } x \to \infty \qquad (3)$$

Feynman (1949) numerically integrated the equation with quadratic approximation for the eight different values of the initial slope, and approximated α in between -1.58876 and -1.58874. Kobayashi *et al*. (1955) obtained an improved asymptotic solution and reported $\alpha = -1.588070972$ with great accuracy. Mason (1964) used a rational approximation, which satisfies both asymptotic approximation of Sommerfeld (1932) and initial approximation of Baker (1930) and obtained following analytical approximation:

$$y(x) = \left(\frac{1 + 1.81061x^{\frac{1}{2}} + 0.60112x}{1 + 1.81061x^{\frac{1}{2}} + 1.39515x + 0.77112x^{\frac{3}{2}} + 0.21465x^2 + 0.04793x^{\frac{5}{2}}}\right)^2 \qquad (4)$$

Csavinsky (1968) obtained an approximate analytical solution for the Thomas-Fermi equation using Ritz variational method with a three-parameter-trial function. Moreover, Roberts (1968) presented a one-parameter trial function. Anderson and Arthurs (1968) suggested a better trial function in comparison with Csavinsky and Roberts. Bender *et al*. (1989) introduced a perturbative technique and applied to several ordinary differential equations including the Thomas-Fermi equation. They calculated the α with 13% relative difference from the exact result. Laurenzi (1990) used a similar perturbative method and calculated the initial slope with only 0.03% relative difference from the exact result. Wazwaz (1999) introduced a new non-perturbative analytical approach to solve the Thomas-Fermi equation, which is based on modified decomposition method with Pade approximants. Abbasbandy and Bervillier (2011) have achieved a new level of accuracy. They used Pade-Hankel method to solve the Thomas-Fermi Equation and were able to compute first 22 decimal places of the initial slope as $\alpha = -1.5880710226113753127189 \pm 7 \times 10^{-22}$. Parand *et al*. (2017) introduced an accurate spectral method using fractional order of rational Jakobi functions. Robin (2018) gave an analytical approximation, which was obtained from numerical data provided by Parand *et al*. (2017). Parand and Delkhosh (2017) introduced another spectral method by using fractional order of rational Chebyshev functions and solved the Thomas-Fermi problem with an excellent numerical accuracy of 37 decimal places. The method of Parand and Delkhosh (2017) was further improved recently by Zhang and Boyd (2019). Zhao *et al.* (2021) introduced a hybrid technique using finite volume method and the asymptotic Puiseux series to obtain approximate solution to the Thomas-Fermi equation.

Solving eq. 1 with common integration methods, such as Runge-Kutta method, involves great difficulty. The main reason for that, y is strongly dependant to the initial slope $\alpha = y'(0)$. In order to use such method, an initial guess for α should be chosen in order to numerically integrate eq.1 from $x = 0$. If α is chosen larger than its exact value, y tends to infinity for some finite value of x. On the other hand, if α is chosen smaller that its correct value, y becomes negative for a finite value of x so that the solution becomes complex. These behaviours of the equation were examined in detail by Hille (1970).

Solving eq. 1 with a numerical method such as finite difference method also involves difficulties. Firstly, the problem is a boundary value problem, which is defined on an unbounded interval. Secondly, direct discretization of the eq. 1 results in a system of nonlinear equations. Finally, it is difficult to achieve second order or higher order accuracies, since second derivative and higher order derivatives of y has a pole at $x = 0$.

In this paper, a second order finite difference method is introduced to solve the Thomas-Fermi equation. Suitable coordinate transformations are used in order to achieve a second order accuracy and avoid any error due to domain truncation. By these transformations, semi-infinite interval of the problem is mapped into interval [0, 1). Quasi-linearization method is applied in order to convert the problem to a set of linear system of equations. The aim of this paper is to provide a simple and effective compact finite difference formulation and show the power of mapping to solve problems defined on an unbounded interval.

2. Coordinate Transformation

The Thomas-Fermi equation is a boundary value problem defined on a semi-infinite interval. A common method to solve such problems is called boundary truncation method. In this method, semi infinite interval where $x \in [0, \infty)$ is replaced with $x \in [0, x_\infty)$ where x_∞ is a sufficiently large finite number. However, choosing x_∞ either is based on the experience or requires additional study. Mathematicians developed several techniques to determine x_∞ (Lentini and Keller 1980; de Hoog and Weiss, 1980; Markowich, 1982; Markowich 1983; Fazio 1992). On either case, truncation of the boundary includes some error.

Another approach is to introduce a suitable coordinate transformation, which maps the unbounded interval of the problem into a bounded one. Van de Vooren and Dijkstra (1970) applied coordinate transformations to investigate laminar fluid flow over a flat plate. They change the original interval $x \in [0, \infty)$ into $\xi \in [0, 1.25)$ via following transformation:

$$x = \frac{5\xi}{5 - 4\xi} + 5\xi^2(1 - \xi^2) \tag{5}$$

Grosch and Orszag (1977) used coordinate transformations for several problems such as heat equation, wave equation, fluid dynamics etc., and showed the success of the method for problems where the solution approaches to a constant value at infinity. Fazio and Jannelli (2014) introduced quasi-uniform grid approach, which is based on the coordinate transformations, in order to solve Falkner-Skan fluid flow equation and a structural mechanics problem. They used following transformations to map $x \in [0, \infty)$ into $\xi \in [0,1)$:

$$\xi = 1 - e^{-\frac{x}{c}} \tag{6}$$

$$\xi = \frac{x}{x + c} \tag{7}$$

where c is a control parameter. Eq.s 6 and 7 are called exponential and algebraic maps, respectively. In this study, we introduce following transformations for the Thomas-Fermi Equation:

$$\xi = 1 - e^{-\sqrt{x}} \quad (8)$$

$$\xi = \frac{\sqrt{x}}{\sqrt{x}+1} \quad (9)$$

These transformations map the interval $x \in [0, \infty)$ into $\xi \in [0,1)$.

Eq. 8 is referred fractional order of exponential map (FOEM) while eq. 9 is referred fractional order of algebraic map (FOAM). The term fractional order is due to the fact that $\sqrt{x}$ is used instead of x in the equations. The reason we use $\sqrt{x}$ instead of x is that, the asymptotic approximation of the eq. 1 around $x = 0$ is of the form of power series expansion of $\sqrt{x}$. Due to this behavior of y(x), it is not possible to achieve second or higher order accuracy by using eq.s 6 and 7 (see Ref. 3). There will always be an error dominated by the term $\frac{4}{3}x^{\frac{3}{2}}$.

The FOEM and FOAM convert the Thomas-Fermi equation to the following boundary value problems, respectively:

$$\frac{(1-\xi)^2}{4\ln(1-\xi)}\frac{d^2y}{d\xi^2} + \frac{(1-\xi)[1-\ln(1-\xi)]}{4[\ln(1-\xi)]^2}\frac{dy}{d\xi} + y^{\frac{3}{2}} = 0, y(0) = 1, y(1) = 0 \quad (10)$$

$$\frac{(1-\xi)^5}{4\xi}\frac{d^2y}{d\xi^2} - \frac{(1-\xi)^4 + 3\xi(1-\xi)^3}{4\xi}\frac{dy}{d\xi} + y^{\frac{3}{2}} = 0, y(0) = 1, y(1) = 0 \quad (11)$$

3. Quasi-linearization of the Equations

The quasi-linearization is an effective method for solving nonlinear differential equations. First, Bellman and Kalaba (1965) introduced this method, and used it to solve several nonlinear boundary value problems. It is also frequently used approach to analyze and solve engineering and design problems as in maritime applications. Amromin (2015) investigated bottom ventilated cavitation in seaways with control device of the flow by quasi-linearize the cavity flow, pressure constancy condition as well as momentum for turbulent flow. In another article, Amromin (2018) executed a research on the impact of sea waves on ships as if the bottom cavity acts as a shock absorber, and quasi-linearized the equations to analyze and solve. Kumari and Kukreja (2022) proposed a method, which consists of quasi-linearization of the non-linear terms, to analyze modified long wave equations. Ahmad *et al*. (2017) introduced a method to carry out static deflection analysis of an infinite beam, which requires governing non-linear equations to be quasi-linearized. Pelka *et al.* (2017) presented a study on underwater positioning and communication for the autonomous vehicles, and they use quasi-linearization to estimate the position based on distance.

Discretization of the eq.s 10 and 11 leads to a set of nonlinear algebraic equations, which are not easy to solve. Instead, we apply quasi-linearization before discretizing the equations in order to obtain a set of linear equations, which can be solved.

In this paper, the Thomas- Fermi equation is quasi-linearized as:

$$\frac{d^2y_{n+1}}{dx^2} - 1.5\sqrt{\frac{y_n}{x}}\,y_{n+1} = -0.5\frac{y_n^{\frac{3}{2}}}{\sqrt{x}} \quad (12)$$

with the boundary conditions:

$$y_{n+1}(0) = 1,\ y_{n+1}(\infty) = 0 \quad (13)$$

where n denotes the number of iteration. The same quasi-linearization could be seen in Mandelzweig and Tabakin (2001) and Parand *et al.* (2017). It can be seen from the eq. 12 that $(n+1)$'th solution of y is calculated from nth iteration. Thus, the quasi-linearisation method requires an initial guess of y_0, which can be chosen from physical or mathematical considerations. In this study, initial guess is assumed as follows:

$$y_0(x) = e^{-x} \quad (14)$$

Using the similar approach, eq.s 10 and 11 can be rearranged as follows:

$$\frac{(1-\xi)^2}{4\ln(1-\xi)}\frac{d^2y_{n+1}}{d\xi^2}+\frac{(1-\xi)[1-\ln(1-\xi)]}{4[\ln(1-\xi)]^2}\frac{dy_{n+1}}{d\xi}+1.5\sqrt{y_n}y_{n+1}=-0.5y_n^{\frac{3}{2}} \tag{15}$$

$$\frac{(1-\xi)^5}{4\xi}\frac{d^2y_{n+1}}{d\xi^2}-\frac{(1-\xi)^4+3\xi(1-\xi)^3}{4\xi}\frac{dy_{n+1}}{d\xi}+1.5\sqrt{y_n}y_{n+1}=-0.5y_n^{\frac{3}{2}} \tag{16}$$

with boundary conditions:

$$y_{n+1}(0)=1, y_{n+1}(1)=0 \tag{17}$$

Now, eq.s 15 and 16 can be solved numerically for y_{n+1} under boundary conditions given eq 17. Iterations can be terminated when a desired level of convergence is achieved.

4. Discretization of the Equations via Finite Difference Method

Finite difference method is considered as a popular, simple, yet powerful tool to obtain approximate solutions for nonlinear boundary value problems. Moreover, particularly in marine sciences, naval architecture and ocean engineering, the method is well-respected and utilized by many engineers and designers to cope with analytically unsolvable engineering problems. Lee *et al.* (2011) simulated and analyzed tank sloshing phenomena regarding to the free surface effect by using finite difference method. Jose *et al.* (2017) modeled and simulated non-linear forces due to breaking waves on a mono-pile structure and compared to experimental results, then they showed that finite difference method yields a good agreement with experiments. Mekki and Ali (2013) used finite difference method based on a Crank-Nicholson type discretization to simulate and handle a water wave problem, which appeals to engineers dealing with ships and off-shore structures. Lu *et al.* (2016) applied finite difference method via utilizing Padé approximation to deal with a numerical solution of the propagation of long waves on the surface of water. In addition, researchers developed compact finite difference schemes for solving singular nonlinear boundary value problems (Roul *et al.* 2019, Setia and Mohanty 2021, Chawla *et al.* 1986, Pandey and Singh 1978).

We use a well-known finite difference method to obtain a numerical solution for eq.s 15 and 16. In order to achieve that, we first divide the interval $[0,1)$ into N equally spaced subintervals. Then, we define $\xi_i = ih$ for $i = 0,1,2,\ldots,N$, and h denotes the length of subintervals. For convenience, we define $y_i = y(\xi_i)$. The boundary conditions in eq. 17 corresponds to:

$$y_0 = 1, y_N = 0 \tag{18}$$

Derivatives of y with respect to ξ can be calculated from the central difference formula, which are given by Gerrald (1978):

$$\left.\frac{d^2y}{d\xi^2}\right|_{\xi_i}=\frac{y_{i+1}-2y_i+y_{i-1}}{h^2} \tag{19}$$

$$\left.\frac{dy}{d\xi}\right|_{\xi_i}=\frac{y_{i+1}-y_{i-1}}{2h} \tag{20}$$

The discretization of FOEM yields to:

$$A_i\frac{(y_{n+1})_{i+1}-2(y_{n+1})_i+(y_{n+1})_{i-1}}{h^2}+B_i\frac{(y_{n+1})_{i+1}-(y_{n+1})_{i-1}}{2h}+C_i(y_{n+1})_i=D_i \tag{21}$$

where coefficients are

$$A_i=\frac{(1-\xi_i)^2}{4\ln(1-\xi_i)} \tag{22}$$

$$B_i=\frac{(1-\xi_i)[1-\ln(1-\xi_i)]}{4[\ln(1-\xi_i)]^2} \tag{23}$$

$$C_i = 1.5\sqrt{(y_n)_i} \tag{24}$$

$$D_i = -0.5(y_n)_i^{\frac{3}{2}} \tag{25}$$

Eqs. 21 – 24 can also be written as in the following:

$$A_i(y_{n+1})_{i-1}+B_i(y_{n+1})_i+C_i(y_{n+1})_{i+1}=D_i \tag{26}$$

where

$$A_i = \frac{(1-\xi_i)^2}{4h^2\ln(1-\xi_i)} - \frac{(1-\xi_i)[1-\ln(1-\xi_i)]}{8h[\ln(1-\xi_i)]^2} \quad (27)$$

$$B_i = 1.5\sqrt{(y_n)_i} - \frac{(1-\xi_i)^2}{2h^2\ln(1-\xi_i)} \quad (28)$$

$$C_i = \frac{(1-\xi_i)^2}{4h^2\ln(1-\xi_i)} + \frac{(1-\xi_i)[1-\ln(1-\xi_i)]}{8h[\ln(1-\xi_i)]^2} \quad (29)$$

$$D_i = -0.5(y_n)_i^{\frac{3}{2}} \quad (30)$$

Eqs. 25 – 29 gives N-1 linear equations for N-1 unknown $(y_{n+1})_i$ where the coefficient matrix of the system of equations has tridiagonal banded form so that this system of equations can easily be solved by the Thomas algorithm (Ford 2015).

Application of the same procedure on FOAM leads to following equations:

$$A_i(y_{n+1})_{i-1} + B_i(y_{n+1})_i + C_i(y_{n+1})_{i+1} = D_i \quad (31)$$

where

$$A_i = \frac{(1-\xi_i)^5}{4h^2\xi_i} + \frac{(1-\xi_i)^4 + 3\xi_i(1-\xi_i)^3}{8h\xi_i} \quad (32)$$

$$B_i = 1.5\sqrt{(y_n)_i} - \frac{(1-\xi_i)^5}{2h^2\xi_i} \quad (33)$$

$$C_i = \frac{(1-\xi_i)^5}{4h^2\xi_i} - \frac{(1-\xi_i)^4 + 3\xi_i(1-\xi_i)^3}{8h\xi_i} \quad (34)$$

$$D_i = -0.5(y_n)_i^{1.5} \quad (35)$$

As one can notice that, the discretization of both eq.s 16 and 17 results in a similar system of linear algebraic equations where the coefficient matrix of the equations have a tridiagonal banded form.

5. Results and Discussion

Fig. 1 compares the meshes created with FOEM and FOAM approaches for $N = 10$. It can be seen that both approaches provide higher resolution for small x while lower resolution for large x. This is very beneficial particularly for problems where y closely follow a constant value for large values of x. When the meshes are compared, it is seen that FOEM approach gives slightly higher resolution than FOAM approach when x is small. While FOAM approach gives higher resolution than FOEM approach when x is large.

Figure 1. Comparison of the Meshes Created Using FOEM (Top Frame) and FOAM (Bottom Frame). The last mesh point is at infinity in both cases.

Table 1 lists the calculated results of $\alpha = y'(0)$ using both FOEM and FOAM approaches for increasing values of N. Estimated order of accuracies (p) are also added to the Table 1. The order of accuracies is estimated by:

$$p = \frac{\ln(|\alpha_{1280} - \alpha_N|) - \ln(|\alpha_{1280} - \alpha_{2N}|)}{\ln 2} \quad (36)$$

where α_N is the initial slope calculated using N intervals. It can be said that the results of the both approaches are in a good agreement. The calculated initial slopes obtained from FOEM approach are slightly less than those obtained from FOAM approach. It can also be deduced from the table that the second order of accuracy is achieved by both approximations. Fig. 2 shows the numerical solution obtained using FOEM approach when $N = 40$.

Table 1. Numerical Approximation of α and Estimated Order of Accuracies

N	α_{FOEM}	Relative Error	p_{FOEM}	α_{FOAM}	Relative Error	p_{FOAM}
40	-1.5866617401	-8,87E-04	1.93774	-1.5849416318	-1,97E-03	1.97696
80	-1.5877020899	-2,32E-04	2.01871	-1.5872738147	-5,02E-04	2.03099
160	-1.5879788813	-5,80E-05	2.05932	-1.5878736628	-1,24E-04	2.08197
320	-1.5880478088	-1,46E-05	2.31679	-1.5880220892	-3,08E-05	2.32841
640	-1.5880651998	-3,67E-06	∞	-1.5880588486	-7,67E-06	∞
1280	-1.5880695670	-9,17E-07		-1.5880679870	-1,91E-06	

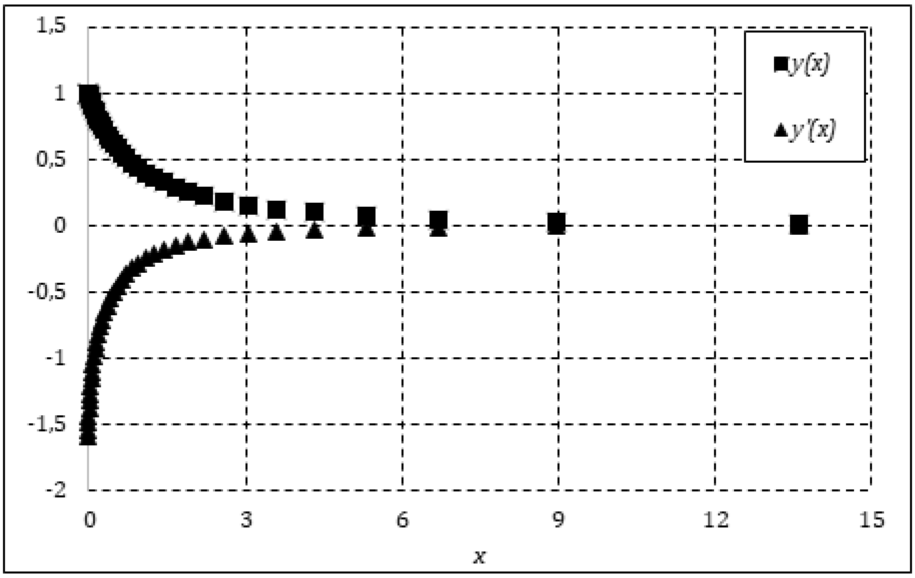

Figure 2. Numerical Solution obtained with FOEM approach ($N = 40$).

Zhang and Boyd (2019) gives $\alpha = -1.5880710226\cdots$ with high accuracy. The error of the both approaches in this paper, when $N = 1280$, is less than 10^{-5} in comparison of initial slope. This error can be reduced by improving the order of the numerical accuracy via Richardson (1927) extrapolation method. Application of this method is explained in detail by Fazio and Janelli (2014). By using this method, extrapolated values of α can be calculated from

$$\alpha_{ext} = \frac{2^p \alpha_{2N} - \alpha_N}{2^p - 1} \qquad (37)$$

Since $p = 2$ for both numerical methods in eq. 36 can be written as

$$\alpha_{ext} = \frac{4\alpha_{2N} - \alpha_N}{3} \qquad (38)$$

Table 2 shows the results obtained for α after extrapolations. We see that the extrapolated value of α is correct up to 10 decimal places for FOEM approach and 8 decimal places for FOAM approach.

Table 2. Numerical Results for α after Richardson's Extrapolations

N	α_{FOEM}	α_{ext}	α_{FOAM}	α_{ext}
320	-1.5880478088		-1.5880220892	
640	-1.5880651998	-1.588070997	-1.5880588486	-1.5880711018
1280	-1.5880695670	-1.588071023	-1.5880679870	-1.5880710332

6. Concluding Remarks

The main goal of this study is to develop an effective numerical method to solve the Thomas-Fermi Equation with second order accuracy. We introduced two different coordinate transformations to convert the semi-infinite interval of the problem to a finite interval in order to avoid potential errors caused by boundary truncation. We applied the quasi-linearization method and the finite difference method to convert the boundary value problem into linear systems of algebraic equations. Resulting algebraic equations are easy to solve since coefficient matrix of them has tridiagonal-banded form. Hence, it can be said that the proposed method requires a low amount of computational effort.

Numerical accuracy of the solution was improved by applying Richardson extrapolation. An alternative to achieve third order or higher order solutions would be to use higher order finite discretization stencils.

Proposed coordinate transformations can be used to solve nonlinear boundary value problems, which are defined on semi-infinite intervals. We suggest following algebraic transformation to extend this method to solve problems defined on $(-\infty, +\infty)$:

$$\xi = \frac{x}{\sqrt{c^2 + x^2}} \qquad 38$$

where c is a control parameter. This transformation converts the infinite interval into (-1, 1).

7. References

Abbasbandy, S. and Bervillier, C., 2011, Analytic continuation of Taylor series and the boundary value problems of some nonlinear ordinary differential equations. *Applied Mathematical Computations,* **218**, 2178–2199.

Ahmad, F., Ullah, M.z., Jang, T.S. and Alaidarous, E.S., 2017, An efficient method for the static deflection analysis of an infinite beam on a nonlinear elastic foundation of one-way spring model, *Ships and Offshore Structures*, **12**, 963-970.

Amromin, E.L., 2015, Ships with ventilated cavitation in seaways and active flow control, *Applied Ocean Research,* **50**, 163–172.

Amromin, E.L., 2018, Ships Bottom Cavities as Shock Absorbers in Waves, *Journal of Marine Science and Application*, **17**, 173–177.

Anderson, N., Arthurs, A.M. and Robinson, P.D., 1968, Variational solutions of the Thomas–Fermi equation, *Nuovo Cimento,* **57**, 523.

Baker, E.B., 1930, The application of the Fermi-Thomas statistical model to the calculation of potential distribution in positive ions, *Physical Reviews,* **36**, 630–647.

Bellman, R.E. and Kalaba, R.E., 1965, *Quasi-linearization and Nonlinear Boundary-Value Problems*, Elsevier Publishing Company, New York.

Bender, C.M., Milton, K.A., Pinsky, S.S. and Simmons, L.M., Jr., 1989, A new perturbative approach to nonlinear problems, *Journal of Mathematical Physics,* **30**, 1447–1455.

Chawla, M.M. and Katti, C.P., 1982, Finite difference methods and their convergence for a class of singular two point boundary value problems, *Numerical Mathematics,* **39**, 341-350.

Chawla, M.M., Mckee, S. and Shaw, G., 1986, Order h^2 method for a singular two-point boundary value problem, *BIT Numerical Mathematics,* **26**, 318-326.

Csavinszky, P., 1968, Approximate Variational Solution of the Thomas-Fermi Equation for Atoms, *Physical Rev*iews, **166**, 53.

de Hoog, F.R. and Weiss, R., 1980, An approximation theory for boundary value problems on infinite intervals, *Computing,* **24**, 227–239.

Fazio, R. and Jannelli, A., 2014, Finite difference schemes on quasi-uniform grids for BVPs on infinite intervals, *Journal Of Computational and Applied Mathematics,* **269**, 14–23.

Fazio, R., 1992, The Blasius problem formulated as a free boundary value problem, *Acta Mechanics*, **95**, 1–7.

Fermi, E., 1928, Eine statistische methode zur bestimmung einiger eigenschaften des atoms und ihre anwendung auf die theorie des periodischen systems der elemente, *Zeitschrift für Physik*, **48**, 73–79.

Feynman, R.P., Metropolis, N. and Teller, E., 1949, Equations of state of elements based on the generalized Fermi-Thomas theory, *Physical Reviews,* **75**(10), 1561–1573.

Ford, W., 2015, *Numerical Linear Algebra with Applications,* Academic Press, Pages 163-179.

Gerald, C.F., 1978, *Applied Num Analysis*, 2.nd Ed., Addison-wesley Publishing Publishing Company, Inc.

Grosch, C.E. and Orszag, S.A., 1977, Numerical solution of problems in unbounded regions: coordinate transforms, *Journal of Computational Physics,* **25**, 273–296.

Hille, E., 1973, Some aspects of the Thomas–Fermi equation, *Journal of Analitical Math*ematics, **23**(1), 147–170.

Josea, J., Choib, S.J., Giljarhusc, K.E.T. and Gudmestada, O.T., 2017, A comparison of numerical simulations of breaking wave forces on a monopile structure using two different numerical models based on finite difference and finite volume methods, *Ocean Engineering*, **137**, 78–88.

Kobayashi, S., Matsukuma, T., Nagi, S. and Umeda, K., 1955, Accurate value of the initial slope of the ordinary T-F function, *Journal of Physical Societies Japan,* **10**, 759–762.

Kumari, A. and Kukreja, V.K., 2022, Sixth order Hermite collocation method for analysis of MRLW equation, Journal of Ocean Engineering and Science, Available online 24 June 2022, https://doi.org/10.1016/j.joes.2022.06.028.

Laurenzi, B.J., 1990, An analytic solution to the Thomas–Fermi equation, *Journal of Mathematical Physics,* **31**, 2535–2537.

Lee, S.H., Lee, Y.G. and LeolJeong, K., 2011, Numerical simulation of three dimensional sloshing phenomena using a finite difference method with marker-density scheme, *Ocean Engineering* **38**, 206–225.

Lentini, M. and Keller, H.B., 1980, Boundary value problems on semi-infinite intervals and their numerical solutions, *SIAM Journal of Numerical Analysis,* **17**, 577–604.

Lu, F., Song, Z. and Zhang, Z., 2016, A Compact Fourth-Order Fınıte Dıfference Scheme For The Improved Boussınesq Equatıon Wıth Dampıng Terms, *Journal of Computational Mathematics,* **34**, 462–478.

Mandelzweig, V.B. and Tabakinb, F., 2001, Quasi-linearization approach to nonlinear problems in physics with application to nonlinear ODEs, *Compuations and. Physical Communications,* **141**, 268–281.

Markowich, P.A., 1982, A theory for the approximation of solution of boundary value problems on infinite intervals, *SIAM Journal Of Mathematical Analysis,* **13**, 484–513.

Markowich, P.A., 1983, Analysis of boundary value problems on infinite intervals, *SIAM Journal Of Mathematical Analysis,* **14**, 11–37.

Mason, J.C., 1964, Rational approximations to the ordinary Thomas–Fermi function and its derivative, *Proceedings of Physical Societies,* **84**, 357–359.

Mekki, A. and Maâtoug M.A., 2013, Numerical simulation of Kadomtsev–Petviashvili–Benjamin– Bona–Mahony equations using finite difference method, *Applied Mathematics and Computation,* **219**, 11214–11222.

Pandey, R.K. and Singh, A.K., 2004, On the convergence of a finite difference method for a class of singular boundary value problems arising in physiology, *Journal Of Computational Applied Mathematics,* **166**.

Parand, K. and Delkhosh, M., 2017, Accurate solution of the Thomas–Fermi equation using the fractional order of rational Chebyshev functions, *Journal of Computations and Applied Mathematics* **317**, 624–642.

Parand, K., Mazaheri, P., Yousefi, H. and Delkhosh, M., 2017, Fractional order of rational Jacobi functions for solving the non-linear singular Thomas-Fermi equation, *European Physical Journal Plus*, **132**, 77.

Pelka, M., Mackenberg, M., Funda, C. and Hellbrück, H., 2017, Optical underwater distance estimation, *Oceans* - Aberdeen, 2017, pp. 1-6.

Richardson L.F., 1927, The deferred approach to the limit, *Philosophical Transactions A,* **226**, 299–349.

Roberts, R.E., 1968, Upper- and Lower-Bound Energy Calculations for Atoms and Molecules in the Thomas-Fermi Theory, *Physical Review,* **170**, 8.

Robin, W., 2018, Another rational analytical approximation to the Thomas–Fermi equation. *Journal Of Innovative Technologies Education,* **5**(1), 7–13.

Roul, P., Goura, V.P. and Agarwal, R., 2019, A compact finite difference method for a general class of nonlinear singular boundary value problems with Neumann and Robin boundary conditions. *Applied Mathematical Computations*, **350**, 283–304.

Setia, N. and Mohanty, R.K., 2021, A third-order finite difference method on a quasi-variable mesh for nonlinear two point boundary value problems with Robin boundary conditions. Soft Computing, ***25***(20), 12775-12788.

Sommerfeld, A., 1932, Asymptotische integration der differentialgleichung des thomas fermischen atoms, *Zeitschrift für Physik,* **78**, 283–308.

Thomas L.H., 1927, The calculation of atomic fields, *Mathematics Proceedings Cambridge,* **23**, 542–548.

van de Vooren and A.I., Dijkstra, D., 1970, The Navier–Stokes solution for laminar flow past a semi-infinite flat plate, *Journal of Engineering Mathematics,* **4**, 9–27.

Wazwaz, A.M., 1999 The modified decomposition method and Pade approximates for solving the Thomas–Fermi equation, *Applied Mathematics and Computation,* **105**, 11–19.

Zhang, X. and Boyd, J.P., 2019, Revisiting the Thomas–Fermi equation: accelerating rational Chebyshev series through coordinate transformations. *Applied Numerical Mathematics,* **135**, 186–205.

Zhao, T., Zhang, Z. and Wang, T., 2021, A hybrid augmented compact finite volume method for the Thomas–Fermi equation. *Mathematics and Computers in Simulation*, **190**, 760-773.