

# NUMEROV'S METHOD FOR APPROXIMATING SOLUTIONS TO POISSON'S EQUATION

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## Abstract

In this paper, a computational approach is taken in trying to solve Poisson's equation. Poisson's equation is often notoriously difficult to solve analytically, so a reliable numerical method has to be established. A Numerov's sixth order approximation scheme was used to approximate the solution of Poisson's equation for a system in which the analytical solution was known and then compared to see how much, if any, differences there were between the Numerov approximation and the analytical solution. After confirming this, Numerov's method was applied to a situation in which the analytical solution is not known. It was found that the Numerov approximation provides an excellent approximation for the solution of Poisson's equation.

## 1 Introduction

When trying to find the electric field of some charge distribution, it is often easiest (unless symmetry allows for the use of Gauss's law) to find the potential,  $V$ . The potential can be found by utilizing the formula

$$V(\vec{r}) = \frac{1}{4\pi\epsilon_0} \int \frac{1}{z} \rho(\vec{r}') d\tau'. \quad (1)$$

Where  $z$  is the vector from a source point ( $\vec{r}'$ ) to the field point ( $\vec{r}$ ). It is more generally kept as  $\vec{r} - \vec{r}'$ , but  $z$  is more compact[1, p. ix]. This integral is often difficult to evaluate analytically[1, p.110]. In addition, in problems that involve conductors, the value of the charge density,  $\rho$  may not be known in advance. In these sorts of situations, a different method is used to solve for the potential, Poisson's equation.

$$\nabla^2 V = -\frac{1}{\epsilon_0} \rho. \quad (2)$$

Often, the potential in a region that contains no charge is of interest. For this, we use Laplace's equation

$$\nabla^2 V = 0. \quad (3)$$

Where  $\nabla^2$  is the Laplacian operator.

In solving Poisson's equation, a numerical solution may be used. One of the common numerical methods used to approximate solutions to Poisson's equation is Numerov's method. Numerov's method is often used where when error on the order of  $h^4$  can be significant, where  $h$  is the step size used in the calculations. Therefore this error cannot be ignored, as the fourth order Runge-Kutta method does. The Numerov's method keeps the terms of order  $h^4$  and then drops terms of order  $h^6$  and higher.

## 2 Computational Physics

Numerical methods are a useful and often invaluable tool for solving physical problems. Computational physics involves the use of computers to study situations in physics[2, p. 1]. Using computers in physics often produce results similar to experiments performed in a laboratory. However, there are some distinct advantages to the use of numerical simulations over performing experiments in the lab. Some of these advantages are[2, p. 2]

- The use of computers allows one to easily test and validate models.
- Computational methods allow for an easier way to catalogue and understand observations.
- The use of computers allows for parameters to be varied in an experiment with far greater ease than could be done in a laboratory. For example, in testing free fall, it is currently not feasible to vary the acceleration due to gravity to see how it affects the experiment. However, it can be easily varied using a computer simulation.
- Computational methods allow for the variation of a single parameter with far more ease than is possible in a laboratory. It is fairly simple to vary only what the scientist wants to vary in a numerical simulation, while in the laboratory, with an experimental setup, varying one thing will often affect other parameters to change, so any difference in the experiment may not be exactly from what the scientist wants to study.
- In general, the use of computer simulations are safer, easier, and most importantly, cheaper, than performing experiments in a laboratory.

Many of the most common problems in physics involve differential equations. In fact, most natural laws relate some quantity to its rate of change with respect to time or space[2, p. 31]. Solving differential equations numerically has one difference from solving differential equations analytically. When solving differential equations analytically, one does not have to know the initial conditions of the situation, a solution up to an arbitrary constant is sufficient, in fact, this is often preferred over a specific solution, as a general solution can be applied to any initial conditions.

When solving differential equations numerically knowing the differential equation of the situation is not enough, one also has to know the value of the solution of the differential

equation at some boundary[3, p. 548]. The most common version of boundary condition is known as the initial value problem where the solution is known at the initial time, and the solution needs to be determined at a different time.

Most techniques that have been developed to solve differential equations involve some sort of iterative technique where the value of solution at a certain time is dependent upon the value of the solution at previous time(s). Most iterative techniques are based upon the Taylor series expansion of the function around the current time  $t_n$ .

$$y_{n+1} = y(t_n + h) = y_n + y'_n \cdot h + \frac{y''_n \cdot h^2}{2!} + \mathcal{O}(h^3), \quad (4)$$

where  $h$  is the step size. One can then solve this expansion for the derivative term that is wanted.

## 2.1 Euler's Method

Euler's method is good for approximating the solutions to equations of the form

$$y' = f(y, t).$$

Euler's method for approximating the solution to differential equations truncates the Taylor series after the second term[2, p. 32].

$$y_{n+1} = y_n + f(y_n, t_n) \cdot h + \mathcal{O}(h^2). \quad (5)$$

This method is prone to error and a relatively small step size is needed to prevent the solution from “blowing up”[4, p. 4]. In general, the smaller the step size is, the better the result will be, however, it comes at a price, the smaller the step size is, the more calculations have to be performed to “travel” a similar distance. For example, instead of iterating from  $t = 0$  to  $t = 100$  with a step size of 1 (which will most likely produce highly substandard results), for a total of 100 steps taken, one could iterate from  $t = 0$  to  $t = 100$  with a step size of 0.01 (which should produce nicer results). This comes at a price, as now 10,000 iterations will have to be performed to cover the same time period. When one uses numerical methods to study differential equations, one has to decide how much accuracy is needed and this decision influences the decision of what step size to use.

## 2.2 Other First Order Approximations

There have been some attempts to improve the Euler method, while still keeping the calculations simple. One such method is known as the Euler-Cromer method[5, p. 5]. The Euler-Cromer method is similar to the Euler method in that it is based off the Taylor expansion. However, when calculating the next step to be taken, the Euler-Cromer method uses the value of the derivative at the point that is of interest, rather than at the point that is currently known, like the Euler method uses. The Euler-Cromer method is given by

$$y_{n+1} = y_n + f(y_n, t_{n+1}) \cdot h + \mathcal{O}(h^2). \quad (6)$$

By using the updated derivative, many of the problems with the Euler method's inaccuracies are fixed[5, p. 5]. Another method that tries to improve the Euler method is known as the Feynman-Newton or half-step method. The Feynman-Newton method uses the value of the derivative halfway between the two end points of the interval. This is given by the equation

$$y_{n+1} = y_n + f\left(y_n, t_{n+\frac{1}{2}}\right) + \mathcal{O}(h^2). \quad (7)$$

This method produces even better results than the Euler-Cromer method does[5, p. 17].

## 2.3 Runge-Kutta Approximation

The Runge-Kutta approximation to the solution of a differential equation is based on taking multiple steps to find the value of the solution at the next location. The most commonly used version of a Runge-Kutta routine is the fourth order Runge-Kutta (often abbreviated RK4). In a fourth order Runge-Kutta routine, four steps are taken between successive time steps. The fourth order Runge-Kutta method is[6, p. 255]

$$y_{n+1} = y_n + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4), \quad (8)$$

where

$$\begin{aligned} k_1 &= h \cdot f(y_n, t_n), \\ k_2 &= h \cdot f\left(y_n + \frac{1}{2}h, t_n + \frac{1}{2}k_1\right), \\ k_3 &= h \cdot f\left(y_n + \frac{1}{2}h, t_n + \frac{1}{2}k_2\right), \\ k_4 &= h \cdot f(y_n + h, t_n + k_3). \end{aligned}$$

The Runge-Kutta fourth order approximation is very reliable, accurate, and quite efficient[2, p. 35]. This method is often as far as is needed to go in approximating differential equations, as long as total accuracy is not needed.

There are numerous other methods that approximate differential equations that could be used. However, they are often based off these methods in one way or another. All of these methods could be done by hand and do not require the use of a computer. However, for a small time step, the amount of work needed to iterate the desired region of interest can require hours of simple calculations to be done by hand. This is where computers are useful. They can take this mindless, repetitive task and perform it far quicker and with less chance for error than a human with a pencil and paper. That is part of the beauty of numerical methods in physics, they often do not require a computer to be done, they just may take a whole lot longer to do without a computer.

### 3 Analytical Solutions to Poisson's Equation

Analytical solutions to Poisson's equation are often messy and complicated, as they can often only be expressed in the form of trigonometric functions, Bessel functions or Legendre polynomials[7, pp 117-119]. Finding these analytical solutions can be time consuming and sometimes can be quite messy.

An example of the complication that can arise in finding the analytical solution is shown in worked example 3.4 from Griffiths **Introduction to Electrodynamics** text. Two infinitely long grounded metal plates at  $y = 0$  and at  $y = a$  are connected at  $x = \pm b$  by metal strips that are maintained at a constant potential,  $V_0$ . The potential inside this rectangular pipe is wanted. Figure 1 shows the situation of interest.

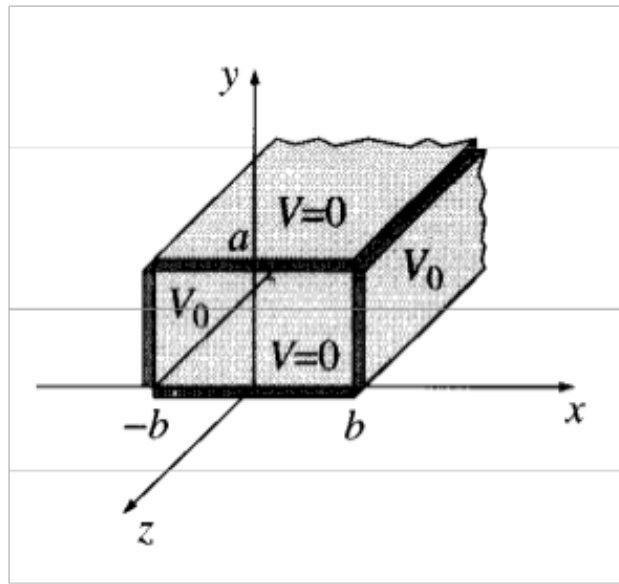


Figure 1: The situation of interest[1, p. 133].

Laplace's equation for this situation is

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0. \quad (9)$$

subject to the boundary conditions

1.  $V = 0$  when  $y = 0$ ,
2.  $V = 0$  when  $y = a$ ,
3.  $V = V_0$  when  $x = b$ ,
4.  $V = V_0$  when  $x = -b$ .

Working through these boundary conditions, the solution, up to a constant that will be determined later, is

$$V(x, y) = \sum_{n=1}^{\infty} C_n \cosh\left(\frac{n\pi}{a}x\right) \sin\left(\frac{n\pi}{a}y\right). \quad (10)$$

By using the third boundary condition, one can solve for  $C_n$  and plug it into this result to obtain the general solution for the potential of this case

$$V(x, y) = \frac{4V_0}{\pi} \sum_{n=1,3,5,\dots}^{\infty} \frac{1}{n} \frac{\cosh\left(\frac{n\pi}{a}x\right)}{\cosh\left(\frac{n\pi}{a}b\right)} \sin\left(\frac{n\pi}{a}y\right). \quad (11)$$

The addition of the third dimension or changing to spherical or cylindrical coordinates adds more complexity to the problem. This is why a reliable numerical approximation scheme is needed for approximating solutions to Poisson's equation.

## 4 Numerov's Method

Numerov's method is used to solve differential equations in the form

$$\frac{d^2y}{dx^2} + k^2(x)y = S(x). \quad (12)$$

Numerov's method is most often used when the error in the calculations of the order  $h^4$  can become significant. Most numerical techniques for ignore error of order  $h^4$ . Numerov's method keeps the terms of order  $h^4$  and then ignores terms of order  $h^6$  and higher[8, p.2] The second derivative can be approximated by the three-point difference formula

$$\frac{y_{n+1} - 2y_n + y_{n-1}}{h^2} = y_n'' + \frac{h^2}{12}y_n'''. \quad (13)$$

where  $y_n''$  is the second derivative and  $y_n'''$  is the fourth derivative, both at the point  $x_n$ . We can rewrite equation 4 (page 3) as

$$y_n''' = \frac{d^2}{dx^2} [-k^2(x)y + S(x)] \Big|_{x=x_n}. \quad (14)$$

We denote  $k(x_n)$  as  $k_n$  and  $S(x_n)$  as  $S_n$  and obtain

$$y_n''' = -\frac{1}{h^2} [k_{n+1}^2 y_{n+1} - 2k_n^2 y_n + k_{n-1}^2 y_{n-1}] + \frac{1}{h^2} [S_{n+1} - 2S_n + S_{n-1}]. \quad (15)$$

by substituting this into equation 4 (page 3) we obtain[9, p.217]

$$\begin{aligned} \left(1 + \frac{h^2}{12}k_{n+1}^2\right) y_{n+1} - 2\left(1 - \frac{5h^2}{12}k_n^2\right) y_n + \left(1 + \frac{h^2}{12}k_{n-1}^2\right) y_{n-1} \\ = \frac{h^2}{12} (S_{n+1} + 10S_n + S_{n-1}), \end{aligned}$$

and then by rearranging and solving for  $y_{n+1}$  we get[10]

$$y_{n+1} = 2y_n - y_{n-1} + \frac{1}{12}h^2 (S_{n+1} + 10S_n + S_{n-1}). \quad (16)$$

the error in Numerov's method is proportional to  $h^6$ , and is better than that of the fourth order Runge-Kutta method[9, p.217]. By applying this to Poisson's equation, one can see that the potential can be determined for a discrete grid by iterating the equation

$$V_{n+1} = 2V_n - V_{n-1} + \frac{1}{12}h^2 (\rho_{n+1} + 10\rho_n + \rho_{n-1}). \quad (17)$$

Let  $V_n = V(x_n)$  be the solution of Poisson's equation at the point  $x_n = a + (n-1)h$  on a grid where  $h$  is an evenly spaced grid.  $h$  is defined as  $h = \frac{b-a}{N}$ [11] where  $b$  and  $a$  are the limits of the area of interest and  $N$  is the number of steps to be taken. Therefore, by knowing the value of the potential at two locations<sup>1</sup> one can then approximate the value of the potential at any other location by iteration.

Another method that could be used to approximate the potential for a region that contains no charge is known as the method of relaxation. In the method of relaxation, the value of the potential at a point  $(x, y)$  is the average of the points around it. To implement the method of relaxation, starting with the values of the potential at the boundaries, and "reasonable" guesses for the values of the potential at the interior points, each pass of the program assigns to each point the value of the mean of its nearest neighbors. After a few iterations, the changes should become negligible and should then provide an approximate solution to Laplace's equation. The method of relaxation follows from the Mean Value and Maximum Value theorems. The Mean Value theorem states that at the center of an included circle (or sphere), the potential is equal to the average of the values of the potential on the surface of the circle[7, p. 116]. The Maximum Value theorem states that the potential cannot have an extrema point anywhere within the region of interest except at the boundary[7, p. 116].

Numerov's method is easily applied to situations where the charge distribution depends on one dimension, for example, a sphere that has a charge density that is only affected by how far from the center of the sphere one is. This is most often denoted as  $\rho(\vec{r}) = k\vec{r}$  where  $\vec{r}$  is the spherical coordinates position vector and  $k$  is an arbitrary constant. The method of relaxation can only be used in regions where there is no charge. The method of relaxation is easily generalized to one, two, or three dimensions.

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<sup>1</sup>Ideally locations that are one step size,  $h$  apart. If the potential is only known at one location, it is customary to use a fourth order Runge-Kutta routine or some other numerical integration that only requires the knowledge of the solution at a single point, rather than two points, to approximate the first step so that two steps can be used in the Numerov's method approximation[8, p4].

## 5 First Step: A Trial

In order to verify the use of Numerov's method, a problem, with a known solution was used. Poisson's equation, equation 2 (page 1), in Cartesian coordinates is

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{\rho}{\epsilon_0}. \quad (18)$$

The charge distribution,  $\rho$ , is chosen to depend only on the distance from the  $x$ -axis, so the  $y$  and  $z$  derivative terms evaluate to be zero, so Poisson's equation for this situation then is

$$\frac{\partial^2 V}{\partial x^2} = -\frac{\rho}{\epsilon_0}. \quad (19)$$

The charge distribution chosen to test the Numerov's method is

$$\rho(r) = e^{-x}. \quad (20)$$

This distribution has the feature that

$$Q_{\text{tot}} = \int_0^\infty e^{-x} dx = 1, \quad (21)$$

In order to make the results easier to understand, the value of  $\epsilon_0$  was set to 1. The exact solution to the problem with the initial condition that  $V(0) = -1$  is

$$V(x) = -e^{-x} - x. \quad (22)$$

The exact solution to the potential is shown in figure 2 (page 9). The results from the Numerov's approximation are shown in figure 3 (page 10) for a step size of  $h = 0.001$ . The percent error of the Numerov's method was calculated. A graph of the percent error for each point is shown in figure 4 (page 11). As figure 4 (page 11) shows, the percent error rises quickly from 0% and then levels off a little above 0.1%.

This low percent error validates the Numerov method so that it can now be used to approximate the solution of more interesting charge distributions. Another method that can be used to judge the difference between the Numerov's method and exact solution is measuring the Cartesian distance between the Numerov's method and exact solution in  $V(x) - x$  space and then dividing that by the value of the exact solution. This provides the percent difference between the exact solution and the Numerov's approximation. This percent difference is given by

$$\% \text{ Diff} = \frac{\sqrt{V_{\text{num}}(x)^2 - V_{\text{exact}}(x)^2}}{V_{\text{exact}}}. \quad (23)$$

This calculation shows how quickly the Numerov's method diverges from the exact solution. The graph of this divergence is seen in figure 5 (page 11). Notice how it appears to diverge then it levels off a certain value. This indicates that the Numerov's approximation diverges quickly from the exact solution, but then levels off to some asymptotic value

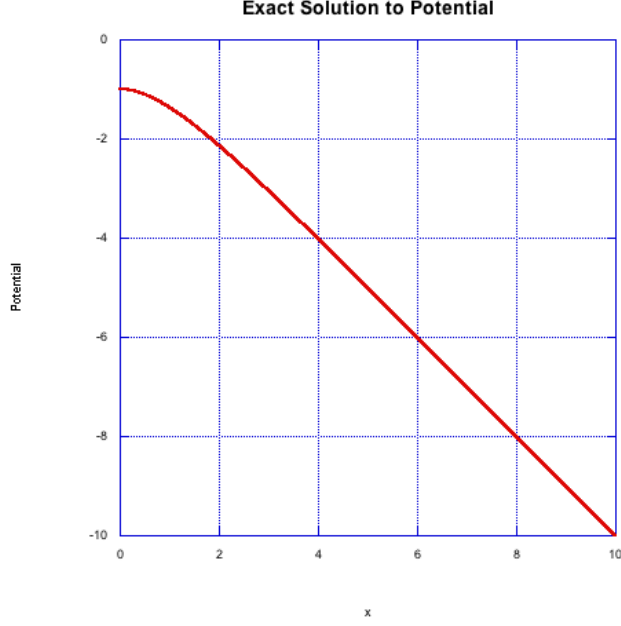


Figure 2: The exact solution to the potential for the charge distribution in equation (22)

## 6 A More Advanced Application

Now that it is known that Numerov's method can produce accurate solutions to Poisson's equation, it was applied to a charge distribution for which the potential is not known in closed form. The charge distribution chosen was

$$\rho(x) = \left( \frac{2}{x^3} - \frac{1}{x} \right) \sin(x) - \frac{2 \cos(x)}{x^2}. \quad (24)$$

This charge distribution has the feature that as  $x \rightarrow \infty$ ,  $\rho(x) \rightarrow 0$  and the total charge enclosed in all space is zero.

$$\int_0^\infty \left( \frac{2}{x^3} - \frac{1}{x} \right) \sin(x) - \frac{2 \cos(x)}{x^2} dx = 0. \quad (25)$$

The results from the Numerov's method approximation are shown in figure 6 (page 12). Notice how the potential immediately shoots up to its maximum value and then starts a sort of decaying oscillation down. Theoretically, as  $x \rightarrow \infty$ ,  $V(x)$  should go to zero. However, in the approximation, the potential fails to settle down to zero, in fact, the approximation shows the potential continuing to decrease in value into negative values.

## 7 Analysis

The Numerov's method was compared to a standard fourth order Runge-Kutta approximation scheme to see if one could get away with using RK4 instead of the more intensive

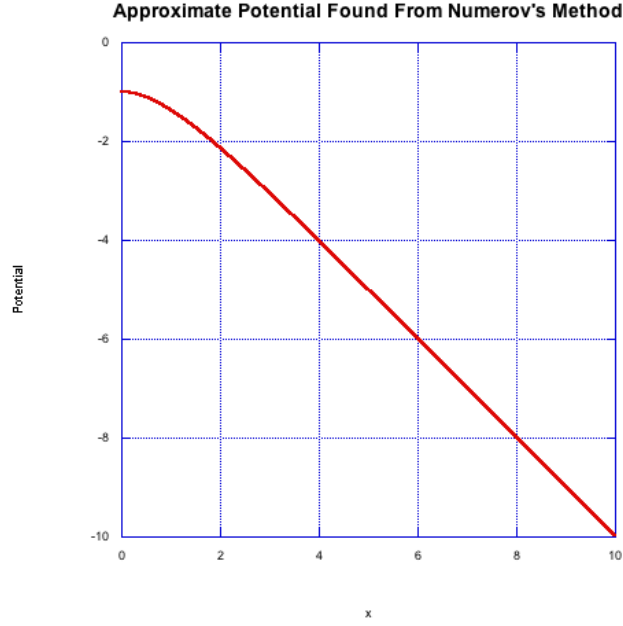


Figure 3: The Numerov's approximation to the potential for the charge distribution in equation 20

Numerov's method. The same charge distribution was used as in the trial of the Numerov's method. In addition, the same step size ( $h = 0.001$ ) was used.

$$\rho(x) = e^{-x}.$$

As figure 7 (page 12) shows, the RK4 approximation is completely inadequate, as it approximates the potential to drop suddenly, and then it jumps up to zero and stays there.

## 8 Conclusions

It has been shown that Numerov's method can be used to model potentials that arise from Poisson's equation. In addition, for a similar step size, Numerov's method provides a far better approximation to the solution than a fourth order Runge-Kutta approximation. Therefore, for instances like solving Poisson's equation, it is better to use Numerov's method than Runge-Kutta or Euler's method. By comparing the percent error for the Numerov's method as well as the percent difference between Numerov's method and the exact solution, it is clearly seen that Numerov's method provides a good approximation to the solution to Poisson's equation.

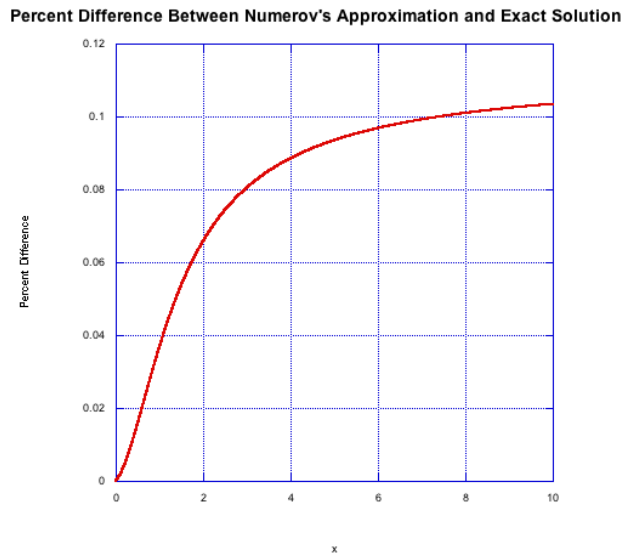


Figure 4: The percent error between the exact solution and the Numerov's approximation to the potential for the charge distribution in equation 20

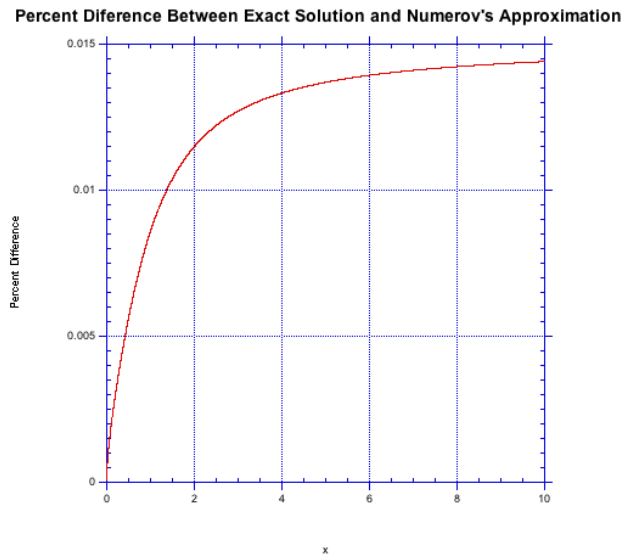


Figure 5: Percent difference between Numerov's method and exact solution

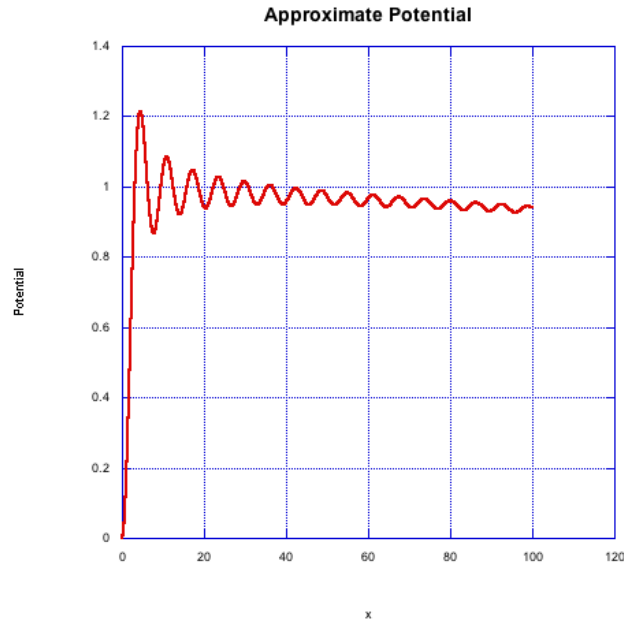


Figure 6: Numerov's method approximation for the potential from the charge distribution in equation 24 (page 9).

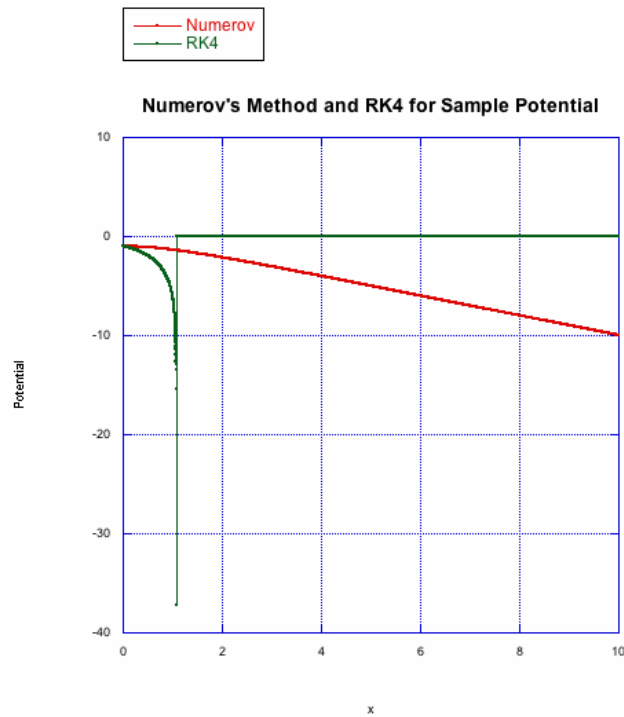


Figure 7: A comparison between Numerov's method and Runge-Kutta fourth order approximation for the sample potential from the charge distribution in equation 20 (page 8)

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## Source Code

PROGRAM Numerov

```
IMPLICIT NONE
INTEGER, PARAMETER :: NumSteps = 100000
REAL*8, PARAMETER :: h = 0.0001d0
INTEGER :: I, J, ErrorStat
REAL*8 :: Initial, FirstStep, Pi, Diff, Exact, Y(2), Time
REAL*8, DIMENSION(1:NumSteps) :: Potential, RKPot
Pi = ACOS(-1.0d0)
OPEN(UNIT = 10, FILE = "Numerov.txt", STATUS = "UNKNOWN", IOSTAT = ErrorStat)
IF (ErrorStat /= 0) STOP "*** ERROR IN OPENING OUTPUT FILE ***"
```

```
Initial = -1.0d0
DO I = 0, NumSteps
    Potential(I) = 0.0d0
    RKPot(I) = 0.0d0
END DO
CALL FindFirstStep(Initial, FirstStep)
Potential(1) = Initial
Potential(2) = FirstStep

DO I = 3, NumSteps
    Potential(I) = Numerovs(I, Potential(I-1), Potential(I-2))
END DO
```

```
DO I = 1, NumSteps
    Exact = ExactS(I)
    Diff = DSQRT(DABS(Potential(I) ** 2 - Exact ** 2))
    WRITE(10,*) I * h, Potential(I), Diff
    Exact = 0.0d0
END DO
```

```
100 FORMAT(1X, A46, 1X)
```

```
! -----
CONTAINS
! -----
```

```
SUBROUTINE FindFirstStep(First, Second)
REAL*8, INTENT(IN) :: First
```

```

REAL*8, INTENT(OUT) :: Second
REAL*8 :: Time, Y(2), Dt
INTEGER :: I
Time = 0.0d0
Dt = h / 1000.0
Y(1) = First
DO I = 0, 1000
    Time = DBLE(I) * DT
    CALL RK4(Y, Time, Dt)
END DO
Second = Y(1)

END SUBROUTINE

```

! -----

```

SUBROUTINE FDT(Y, Time, F)
REAL*8 :: Y(2), F(2), Time

F(1) = Y(2)
F(2) = Rho(Y(1))

```

```

RETURN
END SUBROUTINE FDT

```

! -----

```

SUBROUTINE RK4 (Y, Time, DT)
REAL*8 :: YH(2), Y(2), DT, Y1DT(2), Y2DT(2), Y3DT(2), Y4DT(2), Time
INTEGER :: L
! Calculate k1 = FDT(t, y(t))
CALL FDT(Y, Time, Y1DT)
! -----
! Calculate k2 = FDT(t + DT, y(t)+ 0.5*DT K1)
DO L = 1, 2
    YH(L) = Y(L) + 0.5 * DT * Y1DT(L)
END DO
CALL FDT(YH, Time + DT / 2., Y2DT)
! -----
! Calculate k3 = FDT(t + DT/2, y(t)+ 0.5*DT K2)
DO L = 1, 2
    YH(L) = Y(L) + 0.5 * DT * Y2DT(L)
END DO

```

```

CALL FDT(YH, Time + DT / 2., Y3DT)
! -----
! Calculate k4 = FDT(t + DT, y(t) + dt K3)
DO L = 1, 2
    YH(L) = Y(L) + DT * Y3DT(L)
END DO
CALL FDT(YH, Time + DT, Y4DT)
! -----
! RK4 step
DO L = 1, 2
    Y(L) = Y(L) + (Y1DT(L) + 2. * Y2DT(L) + 2. * Y3DT(L) + Y4DT(L)) * DT / 6.
END DO
END SUBROUTINE RK4

! -----

FUNCTION Rho(r)
REAL*8 :: Rho
Real*8, INTENT(IN) :: r
    Rho = -DEXP(-r)

END FUNCTION

! -----

FUNCTION Numerovs(I, Yn, Ynm1)

REAL*8 :: Numerovs, n, nm1, np1
REAL*8, INTENT(IN) :: Yn, Ynm1
INTEGER, INTENT(IN) :: I
n = h * DBLE(I)
nm1 = h * DBLE(I - 1)
np1 = h * DBLE(I + 1)
Numerovs = (2.0d0 * Yn - Ynm1 + (h ** 2 / 12.0d0) * &
&(Rho(np1)+10.0d0 * Rho(n)+Rho(nm1)))
Rho(n) + Rho(nm1))

END FUNCTION

! -----

FUNCTION ExactS(I)
REAL*8 :: Exacts, x

```

```

INTEGER, INTENT(IN) :: I
x = h * DBLE(I)
Exacts = -DEXP(-x)-x
END FUNCTION

```

```

! -----

```

```

END PROGRAM

```

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