Partial Differential Equations - Lecture 5

1 Introduction

We study differential equations of the form $G\psi = F$ where G is an operator containing differentials, F is a function of the equation variables, and ψ is the solution. When $F = 0$ the equations are homogeneous, otherwise the equation is inhomogeneous. If G has linear form, then the sum of solutions is also a solution. There are two general methods to obtain analytic solutions; 1) an integral equation, and 2) separated variables solution. An example of an integral solution for the partial differential equation in electrostatics (Poisson's equation) is;

$$\nabla^2 V = -\rho/\epsilon$$

$$V(\vec{r}) = \frac{1}{4\pi\epsilon} \int d\tau \, \frac{\rho(\vec{r'})}{\vec{r} - \vec{r'}}$$

In the above, the inhomogeneous term, ρ, is the source (static charge density in this case). Integral equations can be developed from the Green's function which we will study later, however these are not always practical. In the above case, one usually has the value of the potentials on the surfaces of various charge distributions, but not the charge densities that created the potentials in the first place. Thus the above equation is not really a solution but an integral equation.

In general there are an infinite number of solutions to a partial differential equation (pde). Consider the 1-D wave equation;

$$\frac{\partial^2 \psi}{\partial x^2} - (1/v)^2 \frac{\partial^2 \psi}{\partial t^2} = 0$$

Any function which has the relationship between the variables, $x - vt$, is a solution, $\psi(x - vt)$. Thus to find a solution which relates to a specific problem, the boundary conditions (values and/or derivatives of the function) must be applied to obtain a solution. The problem then becomes one of finding the unique solution to the problem which satisfies a specific set of boundary conditions. This is called the boundary problem.

2 Boundary conditions

We look first at possible boundary conditions, and use as an example, the electric potential and its equivalent the electric field. The solution satisfies Poisson's equation, above. Previously we know that the electric field must be perpendicular to a conducting surface, which

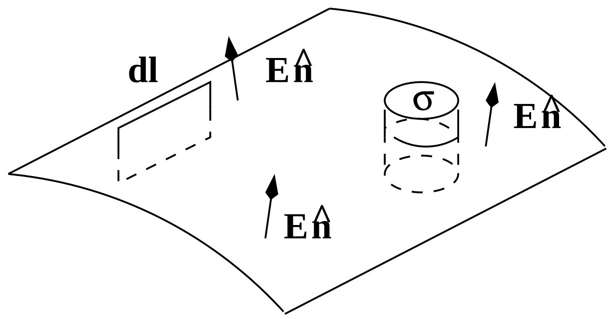

Figure 1: The geometry required to use Gauss' law and Ampere's law to determine the boundary conditions at a conducting surface.

also must vanish within a volume enclosed by a conductor. This means that the potential has constant value on the surface. Figure 1 shows a section of an arbitrary conducting surface with a cylindrical Gaussian surface enclosing a section of the conductor. There is no field within the conductor so no flux penetrates the Gaussian surface inside the volume. Outside the conductor the E field is perpendicular to the surface at the interface. We shrink the dimensions of the Gaussian cylinder so that the outer end cap approaches the surface. The field out of this surface is perpendicular to the area vector and equal to the perpendicular value of E at that point. The flux is then $\vec{E} \cdot \vec{Area} = Q/\epsilon_0$;

$$\vec{E} = (\sigma/\epsilon_0)\,\hat{n}$$

where σ is the surface charge density and $\hat{n}$ is the outward normal. The surface charge on a conductor is given by;

$$\sigma = -\epsilon_0 \vec{\nabla} V \cdot \hat{n}$$

We know that the electric field tangent to a conducting surface vanishes. We now look at this more closely. In Figure 1 there is a drawing of a closed loop that encloses the surface. This loop is called an Amperian loop and we apply reasoning similar to that used for a closed Gaussian surface. In this case we consider the circulation, Γ, of the field around the loop as the loop is reduced to lie near, both above and below, the surface. Thus contributions to the circulation from the edges of the loop vanish as the perpendicular side length approaches zero. This leaves the result;

$$\Gamma = E_{\parallel\, above} dl - E_{\parallel\, below} dl$$

For static charge $\Gamma = 0$ so that $E_{\parallel\, above} = E_{\parallel\, below}$, and for a conductor both of these equal zero.

3 Uniqueness

Now suppose we look for solutions to a second order partial differential equations. The solutions can be determined in several ways, and will usually be represented in the form of a series of special functions obtained from the solutions to a set of eigenvalue equations which satisfy the problem's boundary conditions. Thus the solution may take different forms, and an important question will arise. How do we know that the solution we find is unique? After all, a proper physics solution should have only one answer (*ie* one numerical value when evaluated). There are mathematical proofs which demonstrate unique solutions to various second order differential equations if they satisfy the differential equation and have specified values on a set of boundaries in the geometric space in which the equation applies. These conditions are specified in Table 1.

Table 1: Boundary conditions required for unique solutions to various 2^{nd} order partial differential equations

	Poisson's Eqn $\nabla^2 V = \rho/\epsilon$	Wave Eqn $\nabla^2 V = (1/c^2)\frac{\partial^2 V}{\partial t^2}$	Diffusion Eqn $\nabla^2 V = (1/a)\frac{\partial V}{\partial t}$
Dirichlet			
Open Surface	not enough	not enough	unique
Closed Surface	unique	too much	too much
Neumann			
Open Surface	not enough	not enough	unique
Closed Surface	unique	too much	too much
Cauchy			
Open Surface	unstable	unique	too much
Closed Surface	too much	too much	too much

The Dirichlet boundary conditions require specification of the value of the solution on the boundary. The Neumann boundary conditions require the specification of the derivative of the solution on the boundary. The Cauchy boundary conditions require the specification of both the value of the solution and its normal derivative on the boundary. In the example presented above, we were interested in the solution to Poisson's equation, so we must specify the value of the solution **or** its derivative on a closed surface.

As a very simple example of a solution to Laplace's equation, write the potential between the plates of a parallel plate capacitor as;

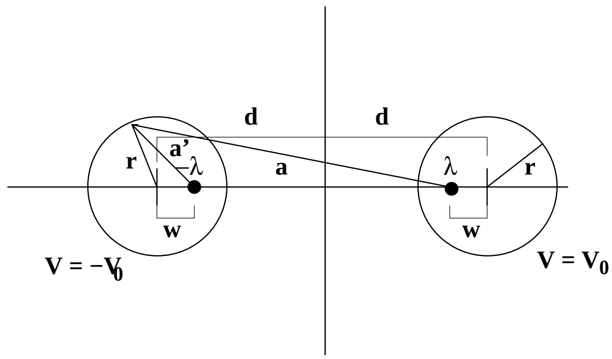

Figure 2: An image charge solution for two conducting cylinders held at opposite potentials

$$V \; = \; -V_0(z/d) \, + \, constant$$

Here d is the distance between the plates and z is the coordinate in this direction so that $z = constant$ represents the potential on the lower plate and $z = d$ the potential on the upper one. This is a solution to Poisson's equation and also satisfies the boundary condition since $\vec{E}$ is perpendicular to the plates. This is the Neumann boundary condition applied on a closed boundary, as the space between the plates extends to ∞ in both directions in (x, y). The above function for V satisfies Poisson's equation and the boundary conditions, so by the uniqueness theorems given in above table, this is the unique solution to the problem.

4 Images

In the lecture on analytic mapping in the complex plane we discussed the development of images in 2-D coordinates. We now have a uniqueness theorem which shows why an analytic map provides an electrostatic solution. The analytic map must satisfy Poisson's equation in 2-D by the Cauchy-Riemann conditions. Then if the uniqueness theorem is satisfied for a proposed function, we have found the unique representation of the solution.

As an example, look at Figure 2. This represents two infinite, conducting cylinders which are chosen to have potentials V_0 and $-V_0$ on their surfaces. We want to find the potential everywhere in space, and to do this we can apply the method of images. We replace the cylinders by image line charges λ and $-\lambda$ as shown. This problem can be worked in the 2-D of the figure because of the symmetry. Recall that the potential of a line charge is;

$$V \; = \; \frac{\lambda}{2\pi\epsilon_0} \, ln(a)$$

Here a is the distance from the line charge to the field point, P. From the figure, the potential at the position of the cylindrical surface of the left cylinder is;

$$V_T = \frac{\lambda}{2\pi\epsilon_0}[ln(a) - \ln(a')] = \frac{\lambda}{2\pi\epsilon_0}[ln(a/a')]$$

From the $\vec{r'} = (2d \vec{-} w) + \vec{a}$ and $\vec{a} = \vec{r'} - (2d \vec{-} w)$. Then;

$$a'^2 = r'^2 + w^2 - 2r'w\,cos(\theta) = r'^2[1 + (w/r')^2 - 2(w/r')\,cos(\theta)]$$

$$a^2 = r'^2 + (2d-w)^2 - 2r'(2d-w)\,cos(\theta) = (2d-w)^2[1 + (r'/(2d-w))^2 - 2(r'/(2d-w))\,cos(\theta)]$$

Substitution gives for the potential gives

$$V_T = \frac{\lambda}{2\pi\epsilon_0}[ln[(2d-w)/r'] + (1/2)\,ln[\frac{1 + (r'/(2d-w))^2 - 2(r'/(2d-w))\,cos(\theta)}{1 + (w/r')^2 - 2(w/r')cos(\theta)}]$$

The location of the center point of the left cylinder is;

$$\vec{r'} = \vec{w} + \vec{a'} \text{ and } \vec{a'} = \vec{r'} - \vec{w}$$

$$\vec{r'} = (2d \vec{-} w) + \vec{a} \text{ and } \vec{a} = \vec{r'} - (2d \vec{-} w)$$

Then;

$$a'^2 = r'^2 + w^2 - 2r'w\,cos(\theta) = r'^2[1 + (w/r')^2 - 2(w/r')\,cos(\theta)]$$

$$a^2 = r'^2 + (2d-w)^2 - 2r'(2d-w)\,cos(\theta) = (2d-w)^2[1 + (r'/(2d-w))^2 - 2(r'/(2d-w))\,cos(\theta)]$$

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The second term on the right vanishes if;

$$(r'/(2d-w)) = w/r'$$

$$w = d \pm \sqrt{d^2 - r'}$$

The potential over the cylinder defined by the radius r' is then a constant value given by;

$$V_T = \frac{\lambda}{2\pi\epsilon_0}[ln[(2d-w)/r']$$

The potential on the right cylindrical surface is the negative of this value.

5 Separation of Variables

We wish to find analytic solutions to linear, homogeneous, second order pde's. The standard technique for finding an analytic solution to this type of equation is to use separation of variables. That is, to assume a solution in the form of $X(x)Y(y)Z(z)$ - a product of separate functions of x, y, and z. Clearly not all solutions can be put in this form. The technique is only useful if there is a coordinate system which matches the boundaries of the problem. That is, if surfaces of a constant variable are the surfaces on which the boundary conditions can be applied. If this is true, the solution can be placed in separable form on the boundary and the boundary condition applied for the variable which specifies the boundary. For Poisson's equation the possibility of obtaining a separable solution occurs for a small number of coordinate systems. These are listed in Table 2. However, just because a separable solution can be found does not mean separable boundary conditions are possible.

Table 2: Coordinate systems in which Laplace's equation separates. To find a solution one must apply the boundary condition on a surface defined when one variable is constant.

Coordinate System	Variables
Cartesian Coordinates	(x,y,z)
Circular Cylindrical Coordinates	(r, ϕ, z)
Elliptic Cylindrical Coordinates	(η, ϕ, z)
Parabolic Cylindrical Coordinates	(μ, ϕ, z)
Spherical Coordinates	(r, θ, ϕ)
Prolate Spheroidal Coordinates	(η, θ, ϕ)
Oblate Spheroidal Coordinates	(η, θ, ϕ)
Parabolic Spheroidal Coordinates	(μ, θ, ϕ)
Conical Coordinates	(r, θ, λ)
Ellipsoidal Coordinates	(r, θ, λ)
Paraboloidal Coordinates	(μ, ν, λ)

There are a few other systems not listed in the table which allow R separation. R separation means the equations separate for one or two of the variables, but not all 3. We found a solution by images for a system of two long conducting cylinders where the solution is independent of z. The solution to this problem can be found in Bi-cylindrical Coordinates which is R separable. Such coordinates can be used if symmetry can be applied to automatically remove one or two of the coordinate variables from the solution. In the Bi-cylindrical coordinates, (r, θ, z), separation occurs when the solution is independent of z, see

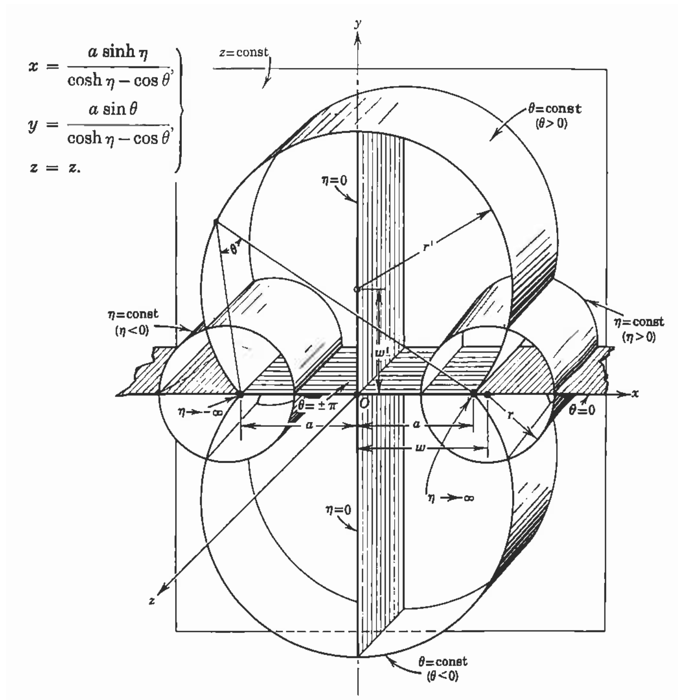

Figure 3: The geometry of Bi-cylindrical coordinates which is R separable

Figure 3. All of the coordinate systems listed in the table are 3-dimensional and orthogonal.

In bicylindrical coordinates the metric is;

$$g_{11} = g_{22} = \frac{a^2}{(cosh(\eta) - cos(\theta))}$$

$$g_{33} = 1$$

These can be substituted into the 2-D Laplace equation to obtain;

$$\frac{\partial^2 V}{\partial \eta^2} + \frac{\partial^2 V}{\partial \theta^2} = 0$$

When separation of variables is applied, one obtains a set of 2^{nd} order ordinary differential equations (ode) of the form;

$$\frac{d}{dz}\,[p(z)\frac{d\eta}{dz}] + [q(z) + \lambda\, r(z)]\eta = 0$$

In the above z is a general variable not a coordinate and $\eta = \eta z$. Also λ is a constant of separation and p, q, r are functions which depend on the coordinate system. The solution which represents a specific physical problem is obtained by applying the boundary conditions. This specifies a discrete but infinite set of the separation constants, λ_n, and solutions,

$\eta_n(z)$. The solution to the ode we seek can then be constructed from this set of functions. The problem of finding a solution to the ode subject to boundary conditions is called the Sturm-Liouville problem.

6 Example in Cartesian Coordinates

A simple example illustrates the eigenvalue solution to the ode which is used to find a representation to the function $F(z)$ given in figure 4. We seek a solution to the equation below in Cartesian Coordinates ;

$$\nabla^2 V = 0$$

$$V = X(x)Y(y)Z(z)$$

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = 0$$

Since each of the above terms are linearly independent as they depend only on linearly independent coordinates, we set each in sequence equal to a constant. This results in 3 equations of the form;

$$\frac{d^2\,\eta}{dz^2} + \lambda\,\eta = 0$$

In the above equation λ is the separation constant and there are two independent separation constants which are used to satisfy the boundary conditions. Comparison to the ode of the general Sturm-Liouville equation written above, $p(z) = r(z) = 1$ and $q(z) = 0$ The 2 independent solutions take the form;

$$\eta(z) = A \begin{pmatrix} sin(\lambda z) \\ cos(\lambda z) \end{pmatrix}$$

Now we apply a boundary condition, for example choose $0 \leq z \leq 2\pi/k$ from the Figure 4. Then $\lambda_n = nk$. We find the expansion coefficients, A_n, using the orthogonality of the eigenfunctions as follows. We ask for a solution;

$$F(z) = \sum A_n\, sin(nkz)$$

Multiply both sides by the eigenfunction $sin(mkz)$ and integrate over$0 \leq z \leq 2\pi/k$. The use orthogonality;

$$\int_0^{2\pi/k} dz\, F(z)\, sin(mkz) =$$

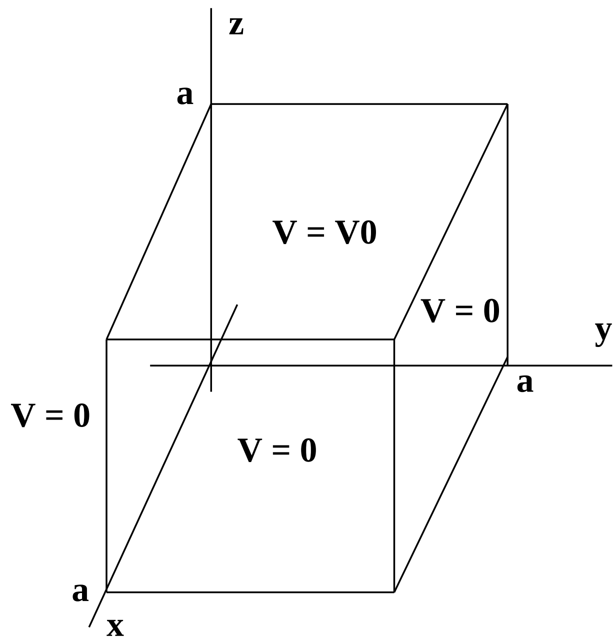

Figure 4: The function to be represented in Cartesian eigenvalues for $0 \leq z \leq 2\pi/k$

$$\sum A_n \int_0^{2\pi/k} dz \, sin(mkz) \, sin(nkz) \; = \; A_m \pi/k$$

Thus;

$$A_m \; = \; (k/\pi) \int_0^{2\pi/k} dz \, F(z) \, sin(mkz)$$

Insert $F(z) \; = \; (k/2\pi)z \; - \; 1/2$ and integrate to obtain;

$$A_m \; = \; -(1/m\pi)$$

Figure 5 shows how the representation of the function is built up as the eigenfunctions are added. Note in particular the convergence to the mean value at the discontinuity.

7 Separation of Variables for Laplace's equation in Spherical Coordinates

In spherical coordinates Laplace's equation is obtained by taking the divergence of the gradient of the potential. As we previously developed, this is;

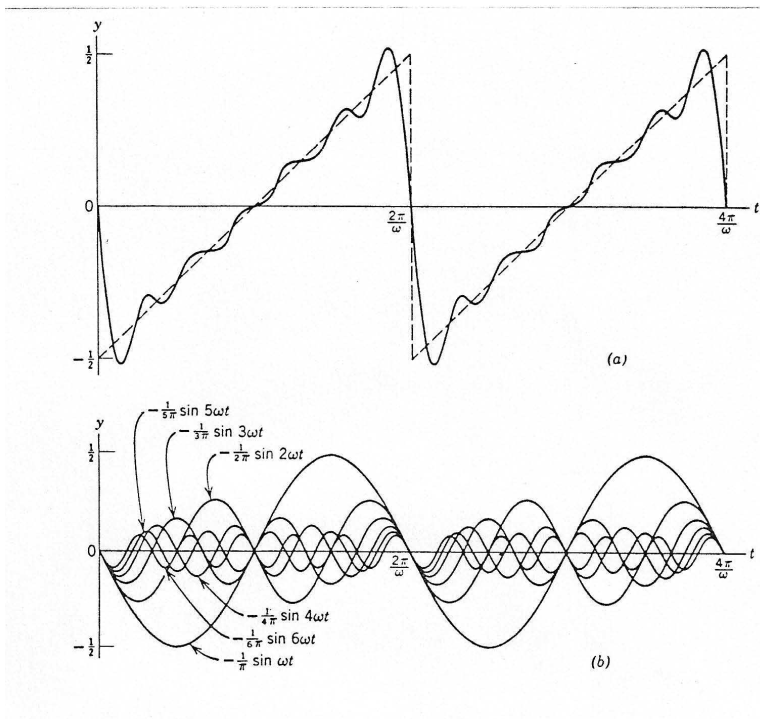

Figure 5: Convergence to the function shown in figure. Note convergence to the mean value at the discontinuity.

$$\nabla^2 V \,=\, (1/r^2)[\frac{\partial}{\partial r}(r^2 \frac{\partial V}{\partial r})] \,+\, (\frac{1}{r^2\, sin(\theta)})[\frac{\partial}{\partial \theta}(sin(\theta)\,\frac{\partial V}{\partial \theta})] \,+\, (\frac{1}{r^2\, sin^2(\theta)})\,[\frac{\partial^2 V}{\partial \phi^2}] \,=\, 0$$

We attempt to obtain a solution by separation of variables. Thus assume that $V = \mathcal{R}(r)\Theta(\theta)\Psi(\phi)$ Substitution into Laplace's equation and then division by V gives;

$$\frac{sin^2(\theta)}{\mathcal{R}}\,\frac{\partial}{\partial r}(\frac{r^2 \partial \mathcal{R}}{\partial r}) \,+\, \frac{sin(\theta)}{\Theta}\,\frac{\partial}{\partial \theta}(\frac{sin(\theta)\partial \Theta}{\partial \theta}) \,+\, \frac{1}{\Psi}\frac{\partial^2 \Psi}{\partial \phi^2} \,=\, 0$$

As with separation in Cartesian coordinates, we isolate terms that depend on only one variable, and because the variables can take on arbitrary values, these terms must equal a constant. In the above we then note that;

$$\frac{1}{\Psi}\frac{d^2\Psi}{d\phi^2} \,=\, -m^2$$

$$\frac{d^2\Psi}{d\phi^2} \,+\, m^2\Psi \,=\, 0$$

Here m^2 is a separation constant. The equation takes the form of an eigenvalue equation with the boundary condition that the function Ψ must repeat as ϕ circles beyond 2π. Because the solution is harmonic this means m must be integral forming harmonic eigenvalues and eigenfunctions.

$$\Psi \,=\, A\, e^{\pm i m \phi}$$

The geometry is 3 dimensional so there will be 2 eigenvalue equations. We have found one with separation constant m^2. Now we separate the terms in r and θ. These result in the two equations;

$$(1/\mathcal{R})\,\frac{d}{dr}(r^2 \frac{d\mathcal{R}}{dr}) \,=\, l(l+1)$$

$$(\frac{1}{\Theta\, sin(\theta)})\frac{\partial}{d\theta}(\frac{sin(\theta) d\Theta}{d\theta}) \,-\, \frac{m^2}{sin^2(\theta)} \,=\, -l(l+1)$$

In the above $l(l+1)$ is the separation constant chosen to have this particular form for convenience as will be seen later. The equation for Θ will become an eigenvalue equation when the boundary condition that $0 < \theta < \pi$ is applied. We will find that l must be integral. The radial equation for $\mathcal{R}$ cannot be an eigenvalue equation, and l and m are specified by the other two equations, above. The radial equation has the following form if we let $U = r\mathcal{R}$;

$$\frac{d^2 U}{dr^2} \,-\, \frac{l(l+1)}{r^2}\, U \,=\, 0$$

This has solutions;

$$U \,=\, Ar^{l+1} \,+\, Br^{-l}$$

$$\mathcal{R} \,=\, Ar^l \,+\, Br^{-(l+1)}$$

Note that every 2^{nd} order differential equation has 2 linearly independent solutions. Now return to the equation for Θ. To simplify the equation make the substitution $x = cos(\theta)$. This then results in the equation;

$$\frac{d^2\Theta}{dx^2} \,-\, \frac{2x}{1-x^2}\,\frac{d(\Theta)}{dx} \,+\, [\frac{l(l+1)}{1-x^2} - \frac{m^2}{(1-x^2)^2}]\Theta \,=\, 0$$

This is the associated Legendre equation which has associated Legendre polynomials as solutions. In problems with axial symmetry, the solutions are independent of ϕ so that $m = 0$. In this later case, solutions to the above equation, are the Legendre polynomials.

8 The Method of Frobenius

Return to Legendre's equation with $m = 0$;

$$\frac{d^2\Theta}{dx^2} \,-\, \frac{2x}{1-x^2}\,\frac{d\Theta}{dx} \,+\, [\frac{l(l+1)}{1-x^2}]\Theta \,=\, 0$$

We look for a series solution of the form;

$$\Theta \,=\, \sum_{n=0}^{\infty} a_n\, x^{n+s}$$

The coefficients a_n are to be chosen to satisfy the ode. The series is assumed to begin with the s^{th} power of x. Put the above series into the ode above to get;

$$(1-x^2)\sum a_n\,(n+s)(n+s-1)\,x^{n+s-2} - \\ 2x\sum a_n(n+s)\,x^{n+s-1} \,+ l(l+1)\,\sum a_n\,x^{n+s} \,=\, 0$$

We then re-order the sums to contain the same power of x. The terms in powers of x are linearly independent, which means the coefficients of each power of x must be independently equal zero. For the lowest two orders of x this has 2 possibilities;

$$s(s-1) \,=\, 0 \text{ if } a_0 \neq 0 \text{ here set } n = 0$$

$$s(s+1) \,=\, 0 \text{ if } a_1 \neq 0 \text{ here set } n = 1$$

Thus we may choose either $a_0 = 0$ or $a_1 = 0$, but of course not both. From the above, if we choose $a_1 = 0$ then we must choose $s = 1$ and only even powers of x will be generated. If we choose $a_0 = 0$ then $s = -1$ and only odd powers of x are allowed. This is shown in the recursion equation obtained from the re-ordered sum of powers above.

$$a_{n+2} = \frac{(n+s)(n+s+1) - l(l+1)}{(n+s+2)(n+s+1)} a_n$$

There is then one unknown constant depending on whether the series is in even or odd powers of x, a_0 or a_1. These form 2 different series solutions. Inspection of the terms of the series shows that it converges for $|x| < 1$. However when $x = \pm 1$ the series does not converge, yet we want a solution also for $\theta = 0$ or π. This can happen if the series does not run to infinity but terminates at some value of n because higher values of n will also equal zero when applying the recursion equation. Then for odd powers, $s = 1$, the series can be terminated if $n = (l-1)$

$$a_{n+2} = \frac{(n+1)(n+2) - l(l+1)}{(n+3)(n+2)} a_n$$

If we want even powers of x then we choose $s = -1$ and to terminate the series we need $n = l + 1$

$$a_{n+2} = \frac{n(n-1) - l(l+1)}{(n+1)n} a_n$$

This generates the Legendre polynomials. Note here that this specifies l as an integer in an eigenvalue equation.

However, be careful here. There are problems that exclude the z axis and the infinities at $x = \pm 1$ were used to create an eigenfunction equation and restrict the solutions to the Legnedre polynomials. The Legendre polynomials are not always sufficient to expand an arbitrary function which does not include $x = \pm 1$. A second order ode has 2 linearly independent solutions, so there is another set of solutions which are infinite at $x = \pm 1$, and must be used in those problems. We do not consider this now.

9 Example

As an example, consider Bessel's equation with solution $y(x)$;

$$x^2 y'' + x y' + (x^2 - j^2) y = 0$$

For future reference this equation has a regular singular point at $z = 0$ and an irregular point at ∞. Use the following series expansions for the solution;

$$y = \sum a_n \, x^{n+s}$$

$$y' = \sum a_n(n+s)x^{n+s-1}$$

$$y'' = \sum a_n(n+s)(n+s-1)x^{n+s-2}$$

Substitute into the equation and collect powers of x. The indicial equation occurs for the lowest powers of x. There are two possibilities.

1) $a_0[s(s-1) + s - j^2] = 0$

2) $a_1[s(1+s) + (s+1) - j^2] = 0$

For equation 1 we can choose $s = \pm j$ or $a_0 = 0$

For equation 2 we can choose $s = -1 \pm j$ or $a_1 = 0$

We obtain a series solution for $s = j$ and $a_1 = 0$. However if we choose $s = -1 + j$ and $a_0 = 0$ the same series results. The reason we do not get a 2^{nd} solution is the attempt to expand about the singular point $x = 0$. Thus one must reduce the level of the singularity by a change of variable. The second solution has a logarithmic behavior as $x \to 0$. The issue of singularities is discussed in the next section.

10 General Properties of Series Solutions

In the separation of the Helmholtz equation which is an ode of the form;

$$\frac{d^2\psi}{dz^2} + p(z)\frac{d\psi}{dz} + q(z)\psi = 0$$

the functions $p(z)$ and $q(z)$ are simple algebraic functions of z containing a finite number of poles. A pole here is a singularity of the form $\frac{1}{(z-a)^n}$ with n an integer. The general solution will have singularities at the poles of the equation. All other points are called "regular points". The solution is regular at regular points which is observed by a power series solution.

Thus we expand the functions p and q about the point $z = a$. This results in;

$$p(z) = p(a) + (z-a)p^{(1)}(a) + \frac{(z-a)^2}{2}p^{(2)}(a) + \cdots$$

Then q and the solution ψ are expanded in the same way, *eg*;

$$\psi_1 = A_0 + A_1(z-a) + A_2(x-a)^2 + \cdots$$

Substitute into the equation and collect terms. Each power of $(z-a)$ must be separately set to zero because the terms are linearly independent. Take the lowest order powers of $(z-a)$.

$$A_2 = -A_1/2\,p(a) \quad \text{if } A_0 = 0$$

Or;

$$A_2 = -A_0/2\,q(a) \quad \text{if } A_1 = 0$$

The result is 2 linearly independent, analytic solutions. This was because p and q are analytic. If p has a pole at $z = a$ and q is analytic, then one solution will be analytic and one will have a singularity. If p has a pole of higher order than first and q a pole of higher order than second, then the equation has an irregular singularity, otherwise the equation has regular singular points. Regular singular points in the equation may be separated in the solution. Thus when attempting to solve a linear ode of unfamiliar form, one should first locate all the singularities. If the singularities are poles one may proceed to find a solution by series. If irregular singularities occur, then attempt to remove them by a change of variable. If this is unsuccessful, one must resort to numerical integration. As previously, the nature of the point at infinity is determined by the variable change $z = 1/w$. When at all possible, put the equation in standard form by change of variable.

1. For 1 Singular Point
   place the point at 0

2. For 2 Singular Points
   place one at 0 and the other ∞

3. For 3 Singular Points
   place the singular points at 0, 1, ∞

4. There is no standard form for higher numbers of singular points

11 Classification of equations

Here we consider only ode resulting from separation of the Helmholtz equation in different coordinate systems. They can be classified by the number and type of singularities.

11.1 One regular singular point

The equation has the form

$$\psi^{(2)} \ + \ \frac{2}{z-a}\psi \ = \ 0$$

There is no singularity at $z = \infty$ as seen by the transformation $z = 1/w$. If the singularity is placed at ∞ the equation simplifies to $\psi^{(2)} \ = \ 0$

11.2 Two regular singular points

The equation has the standard form;

$$\psi^{(2)} + \frac{\lambda + \mu - 1}{z}\psi^{(1)} + \frac{\lambda\mu}{z^2}\psi \ = \ 0$$

The singular points are placed at 0 and ∞. If there is the special case where $\lambda = \mu$ the second solution involves a ln term

11.3 One irregular point

Suppose the equation;

$$\psi^{(2)} + \frac{2}{z-a}\psi^{(1)} \ + \ \frac{k^2}{(z-a)^4}\psi \ = \ 0$$

The term $(z-a)^4$ is responsible for the irregular singular point and the term $\frac{2}{z-a}$ prevents a singular point at ∞. The solution is obtained by placing the irregular point at ∞, $z = 1/w$. This results in the equation;

$$\psi^{(1)} - k^2\psi \ = \ 0$$

The solutions are obviously exponentials.

11.4 Final remarks

One can continue this analysis looking at various combinations of singular points. However, the above examples show the power in looking for, and moving the singularities to simplify the equation and solution. If for no other reason, solutions for standard equations have been studied, and tabulated, and computer algorithms coded to calculate the solutions for most needs. Note the attempt to find series solutions to Bessel's equation. We find one, but need a change of variable to move the singularity in order to get the 2^{nd} linearly independent solution.

12 Linear Independence

Generally there are an infinite number of solutions to pde and ode, but essentially all differ only by a different constant. To be linearly independent a set of functions, ϕ_i, must obey the relation;

$$\sum_i a_1 \phi_i = 0$$

If not all a_1 equal 0 then some subset of the ϕ_i are linearly independent. Suppose the functions, ϕ_i, are linearly independent. Take the derivatives of the above equation;

$$\sum a_i \phi_i^{(0)} = 0$$

$$\sum a_i \phi_i^{(1)} = 0$$

$$\cdots$$

$$\sum a_i \phi_i^{(n)} = 0$$

This represents a set of homogeneous equations for a_i, which may be solved if the determinant;

$$\begin{vmatrix} \phi_1^{(0)} & \phi_2^{(0)} & \cdots & \phi_n^{(0)} \\ \phi_1^{(1)} & \phi_2^{(1} & \cdots & \phi_n^{(1)} \\ & \cdots & & \\ \phi_1^{(n-1)} & \phi_2^{(n-1)} & \cdots & \phi_n^{(n-1)} \end{vmatrix} = 0$$

This determinant is the Wronskian. If it is zero, the equations may be solved for the a_i and the functions, ϕ_i are linearly dependent. If not, the functions are linearly independent. Note that this must occur for the total range of the dynamic variable and not at isolated values.

As an example, second order ode have 2 linearly independent solutions, y_1 and y_2. In this case the Wronskain is $w = y_1 y_2' - y' y_2$. If $w = 0$ then $y_1 = c y_2$ with c a constant, so the functions y_1 and y_2 are linearly dependent. Then suppose we have one solution, y_1. Starting at the point, z_0, build a second solution. Thus let;

$$y_2 = \alpha y_1$$

$$y' = \beta y_1'$$

where $\alpha \neq \beta$. The Wronskin is $w = (\beta - \alpha)\, y_1 y_1'$ at $z = z_0$. For any value of z;

$$\frac{dw}{dz} = y_1 y'' - y'' y_2$$

Assume the ode of the form;

$$y'' + p(z) y' + q(z) y = 0$$

Then by substitution and reduction of terms;

$$\frac{w}{dz} = p(z)\, w$$

Integration gives;

$$w(z) = w(z_0)\, e^{\int_{z_0}^{z} dz\, p(z)}$$

Since $w = y_1 y_2' - y_2 y_1'$, the second solution is;

$$\frac{d}{dz}(y_2/y_1) = (w(z_0)/y_1^2)\, e^{\int_{z_0}^{z} dz\, p(z)}$$

$$y_2/y_1 = w(z_0) \int_{z_0}^{z} dz\, \frac{e^{\int_{z_0}^{z} dz\, p(z)}}{y_1^2}$$

However, one still may ask the question if all solutions can be represented by a linear combination of these two solutions.

$$y_3 = A\, y_1 + B\, y_2$$

The derivative at z_0 allows one to construct the Wronskin;

$$w = y_3 y_1' - y_1 y_3'$$

Use the ode and the definition of y_3 to show that y_3 can be expanded in a Taylor expansion in terms of y_1 and y_2 about the point z_0 so it is a linear combination of y_1 and y_2 and not a linearly independent solution.

13 A final example of a series solution

Suppose the Schrodinger radial equation for the Coulomb ode. This has the form;

$$(1/r^2)\frac{d}{dr}[r^2\frac{dR_l}{dr}] + [k^2 - (2\eta k/r) - l(l+1)/r^2]R_l = 0$$

Let $R_l = \chi_l/r$ and substitute to obtain;

$$(1/r)\frac{d^2\chi_l}{dr^2} + [k^2 - (2\eta k/r) - l(l+1)/r^2]\chi_l/r = 0$$

Finally $\rho = kr$ gives the equation in standard form;

$$\frac{d^2\chi_l}{d\rho^2} + [1 - (2\eta/\rho) - l(l+1)/\rho^2]\chi_l = 0$$

In the above $\eta = \frac{\mu Zze^2}{\hbar k}$ and $k = (\frac{2\mu E}{\hbar^2})^{1/2}$. The charges are Z and z, the reduced mass μ, the momentum in $\hbar$ units, k, and the kinetic energy, E. This is a second order linear ode so there are 2 linearly independent solutions written at $F_l(\eta, \rho)$ and $G_l(\eta, \rho)$. Here F_l is the regular Coulomb wave function, and G_l the irregular one. The equation has been put into standard form where there is a regular singular point at 0 and an irregular singular point at ∞. These singularities appear in the solutions, F_l and G_l respectively. The Coulomb wave function can be expanded in a series of a complete set of functions. The series representation is equivalent to the Confluent Hypergeometric series. To find the series solution make the following substitutions;

$$\chi_l = \sum A_n\, \rho^{n+s}$$

$$\chi_l' = \sum A_n(n+s)\, \rho^{n+s-1}$$

$$\chi_l'' = \sum A_n(n+s)(n+s-1)\, \rho^{n+s-2}$$

The indicial equation is;

$$[s(s-1) - l(l+1)]A_0 = 0$$

Thus we can choose $s = l + 1$ with $A_0 \neq 0$.

$$[n+l][n-(l+1)]A_n^l = 2\eta\, A_{n-1}^l - a_{n-2}^l$$

The series takes the form;

$$F_l(\eta, \rho) = \sum_{n=l+1}^{\infty} A_n^l(\eta)\, \rho^{n-(l+1)}$$

with chosen initial values of the coefficients given by; $A^l_{l+1} \;=\; 1$ and $A^l_{l+2} \;=\; \eta/(l+1)$

14 Numerical Methods

When all else fails or one needs to obtain a numerical answer to a specific problem, a numerical evaluation is possible. However this requires some analysis to determine the type and position of the singularities. The convergence of the numerical method is not guaranteed unless a properly selected region and procedure are employed.

14.1 Numerical Differentiation

The obvious first step is just to find the difference between two values of the function evaluated at nearby points and divide by the difference between the nearby points.

$$\delta\, f(x) \;=\; \frac{f(x+h/2) - f(x-h/2)}{\delta\, x}$$

The definition of the differential of f is taken as the limit as $\delta\, x \to 0$. However, this must be carefully handled as the numerator and denominator approach 0, and accuracy of the differences becomes an issue. Thus, we can look at additional terms in the Taylor expansion of the function, $f(x)$ about the point x_0.

We are to differentiate a function $f(x)$ at x_0. First express $f(x)$ in a Taylor expansion about x_0.

$$f(x) \;=\; f(x_0) + f'(x_0)\,(x - x_0) + f''(x_0)\,\frac{(x-x_0)^2}{2} + f'''(x_0)\,\frac{(x-x_0)^3}{6} + \cdots$$

Here we will let $x = x_0 + h/2$. This then results in;

$$f(x_0 + h/2) \;=\; f(x_0) + f'(x_0)\,\frac{h}{2} + f''(x_0)\,\frac{h^2}{8} + f'''\,\frac{(x_0)\,h^3}{48} + \cdots$$

Then let $h = x_0 - h/2$ to obtain;

$$f(x_0 - h/2) \;=\; f(x_0) - f'(x_0)\,\frac{h}{2} + f''(x_0)\,\frac{h^2}{8} - f'''\,\frac{(x_0)\,h^3}{48} + \cdots$$

Keeping terms only to this order, subtract these equations to obtain;

$$f(x_0 + h/2) - f(x_0 - h/2) \;=\; f'(x_0)\,h + f'''(x_0)\,\frac{h^3}{24}$$

Solving for the derivative;

$$f'(x_0) \;=\; \frac{f(x_0+h/2)-f(x_0-h/2)}{h} \;-\; f'''(x_0)\,\frac{h^3}{24}$$

Rewrite the third order differential in terms of difference equations;

$$f'''(x) \;=\; \frac{f''(x+h/2)-f''(x-h/2)}{h}$$

And

$$f''(x) \;=\; \frac{f(x_0+h)-2f(x_0+h/2)+f(x_0) \;-\; f(x_0)+2f(x_0-h/2)-f(x_0-h)}{h^2}$$

Keeping track of all the variables,and substituting the above, one obtains;

$$f'(x_0) \;=\; \frac{[f(x_0+h/2)-f(x_0-h/2)]}{h}\,[1-\frac{h}{12}] \;-\; \frac{1}{24}\,[f(x_0+h)-f(x_0-h)]$$

As another approach, find a polynomial, $P_m(x)$ having a common first $m+1$ differences with $f(x)$.

$$f_0, \delta f_0, \delta^2 f_0, \cdots\; \delta^{m+1} f_0$$

Let $u=(x-x_0)/h$, and $2k=m+1$. Then use Stirling's interpolation formula;

$f \;=\; f_0 + u(a\delta f_0) + (1/2!)u^2(\delta^2 f_0) + (1/3!)u(u-1)(a\delta^3 f_0) + \cdots + (1/(2k-1)!)\,u(u^2-1)(u^2-4)\cdots[u^2-(k-1)^2](a\delta^{2k-1} f_0) \;+\; (1/2k!)u^2(u^2-1)\cdots[u^2-(k-1)^2](\delta^{2k} f_0)$

In the above a is the average operator. As an example;

$$af \;=\; (1/2)[f(x+h/2)+f(x-h/2)]$$

$$a\delta^3 f \;=\; (1/2)[f(x+2h)-2f(x+h)+2f(x-h)-f(x-2h)]$$

Then ;

$$\frac{df}{dx} \approx (1/h)[\frac{f(x+h)-f(x-h)}{2}] - (1/6)[\frac{f(x+2h)-2f(x+h)+2f(x-h)-f(x-2h)}{2}]$$

Choose $f(x) \;=\; cos(\theta)$ with $\theta = 1.76$, and $h = 0.02$. The value of the function and derivative are, -0.1880768 and -0.9821543, respectively. Evaluate the terms in the approximation to obtain for the derivative, -0.98215625. Even the 1st term is a good approximation in some situations, -0.98209

14.2 Numerical Integration

It is also possible to use polynomials fitted to a function over small sub-intervals to approximate the value of the integral of the function over some range. The accuracy of the resulting integral depends on the interval size, the degree of the polynomial, and the accuracy with which the polynomial fits the function. If the interval is approximated by a 2^{nd} order polynomial (parabolic fit) one obtains Simpson's rule. The integral $\int_a^b dx f(x)$ represents the area under the curve $f(x)$ between $a \leq x \leq b$. This can be approximated by the sum of rectangular areas, $dx\, f(x)$. A better approximation is to choose to fit three points of f(x) to a parabolic curve, as shown in Figure 6. This leads to Simpson's rule for the integral.

$$\int_b^a dx\, f(x) \;=\; h/3([f(a) + f(b)] + 4[f_1 + f_3 + \cdots + f_{n-1}] + 2[f_2 + f_4 + \cdots + f_{n-2}])$$

Note that $f(x)$ is divided into an odd number of evaluation points.

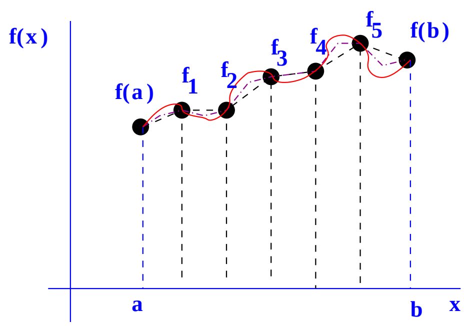

Figure 6: Interpretation of an integral as an area under a curve

As an example, use the integral;

$$I \;=\; \int_0^{\pi/2} dx\, cos(x)$$

with a step size of 0.1. Simpson's rule gives a value for the integral of 1.000001, while the rectangular approximation gives, 1.05505.

14.3 Numerical Solution to Differential equations

Generally the solution starts from a boundary where the value of the function and/or derivatives are known at several initial points. Recall that a unique solution is determined by its boundary conditions. If the equation is separable and boundary conditions can be applied then the solution can be formed by a series of eigenfunctions. There are different techniques which can be applied, some more suitable to specific equation forms than others. In addition, the direction of the integration is sometimes important to maintain stability in the solution. Often the solution is in the form of predictor/corrector equations which improve the numerical value by applying a predictor equation and then a corrector to improve the solution by iteration. A few example methods are given below.

14.3.1 Milne's Method

Suppose the differential equation; $y'' = f(x, y)$, with boundary conditions $y = y_0$, $y' = y'_0$ at $x = x_0$ We then apply Simpson's rule to obtain predictor and corrector forms.

Predictor

$$y_{n+1} = y_n + y_{n-2} - y_{n-3} +$$

$$h^2/4[5y''_n + 2y''_{n-1} + 5y''_{n-2}]$$

Corrector

$$y_n = 2y_{n-1} - y_{n-2} +$$

$$h^2/3[y''_n + 10y''_{n-1} + y''_{n-2}]$$

Note that this method requires 4 starting values.

14.3.2 Numerof Method

The equation has the form; $y'' = f(x)y$

$$y_n = \frac{2y_{n-1} - y_{n-2} + (h^2/12)\, y''_{n-2} + 10(h^2/12)\, y''_{n-1}}{1 - (h^2/12) f(x_n)}$$

This method requires two starting values. As an example we look at the solution to the equation;

$$\frac{d^2y}{dx^2} + k^2\, y = 0$$

The solution has the form;

$$y = A\,sin(kx) + B\,cos(kx)$$

Choose the boundary conditions to be;

$$y = 0 \text{ at } x = 0$$

$$y' = 1 \text{ at } x = 0$$

This gives the solution, $y = sin(kx)$. We integrate the 0de equation using the Numerof method for $0 < x < 2.5$ with $k = 1$ and a step, $h = 0.5$. The result is shown in Figure 7.

14.3.3 Runge-Kutta Method (4^{th} Order)

The differential equations are;

$$y' = F(x, y, u)$$

$$u' = G(x, y, u)$$

Here y, u are known at $x = x_0$. When $F = u$ the coupled problem is $y'' = G(x, y, y')$

We then obtain;

$$y_{n+1} = y_n + hy'_n + (h/6)(m_0 + m_1 + m_2)$$

$$y'_{n+1} = y'_n + (1/6)(m_0 + 2m_1 + 2m_2 + m_3)$$

$$m_0 = hG(x_n, y_n, y'_n)$$

$$m_1 = hG(x_n + h/2, y_n + (h/2)y'_n, y'_n + m_0/2)$$

$$m_2 = hG(x_n + h/2, y_n + (h/2)y'_n + hm_0/4, y'_n) + m_1/2$$

$$m_3 = hG(x_n + h, y_n + hy'_n + hm_1/2, y'_n + m_2)$$

The error in the iteration is $< O(h^5)$. This method is useful for most ode, and can be applied to non-linear equations. Suppose the equation;

X(rad)	y	Sin(x)
.1ØØØØØØE+ØØ	.9983341E-Ø1	.9983342E-Ø1
.15ØØØØØE+ØØ	.1494381E+ØØ	.1494381E+ØØ
.2ØØØØØØE+ØØ	.1986693E+ØØ	.1986693E+ØØ
.25ØØØØØE+ØØ	.2474Ø39E+ØØ	.2474Ø4ØE+ØØ
.3ØØØØØØE+ØØ	.29552Ø1E+ØØ	.29552Ø2E+ØØ
.35ØØØØØE+ØØ	.3428976E+ØØ	.3428978E+ØØ
.4ØØØØØØE+ØØ	.3894181E+ØØ	.3894183E+ØØ
.45ØØØØØE+ØØ	.4349651E+ØØ	.4349656E+ØØ
.5ØØØØØØE+ØØ	.479425ØE+ØØ	.4794255E+ØØ
.55ØØØØØE+ØØ	.5226865E+ØØ	.5226873E+ØØ
.6ØØØØØØE+ØØ	.5646417E+ØØ	.5646425E+ØØ
.65ØØØØØE+ØØ	.6Ø51855E+ØØ	.6Ø51864E+ØØ
.7ØØØØØØE+ØØ	.6442167E+ØØ	.6442177E+ØØ
.75ØØØØØE+ØØ	.6816376E+ØØ	.6816388E+ØØ
.8ØØØØØØE+ØØ	.7173548E+ØØ	.7173561E+ØØ
.85ØØØØØE+ØØ	.751279ØE+ØØ	.75128Ø4E+ØØ
.9ØØØØØØE+ØØ	.7833254E+ØØ	.7833269E+ØØ
.95ØØØØØE+ØØ	.8134139E+ØØ	.8134155E+ØØ
.1ØØØØØØE+Ø1	.8414692E+ØØ	.841471ØE+ØØ
.1Ø5ØØØØE+Ø1	.8674211E+ØØ	.8674232E+ØØ
.11ØØØØØE+Ø1	.89120Ø48E+ØØ	.8912Ø73E+ØØ
.115ØØØØE+Ø1	.91276Ø9E+ØØ	.912764ØE+ØØ
.12ØØØØØE+Ø1	.932Ø356E+ØØ	.932Ø391E+ØØ
.125ØØØØE+Ø1	.94898Ø6E+ØØ	.9489846E+ØØ
.13ØØØØØE+Ø1	.9635536E+ØØ	.9635582E+ØØ
.135ØØØØE+Ø1	.9757182E+ØØ	.9757234E+ØØ
.14ØØØØØE+Ø1	.9854439E+ØØ	.9854497E+ØØ
.145ØØØØE+Ø1	.9927Ø64E+ØØ	.992713ØE+ØØ
.15ØØØØØE+Ø1	.9974875E+ØØ	.997495ØE+ØØ
.155ØØØØE+Ø1	.9997754E+ØØ	.9997838E+ØØ
.16ØØØØØE+Ø1	.9995643E+ØØ	.9995736E+ØØ
.165ØØØØE+Ø1	.9968548E+ØØ	.996865ØE+ØØ
.17ØØØØØE+Ø1	.9916537E+ØØ	.9916648E+ØØ
.175ØØØØE+Ø1	.983974ØE+ØØ	.983986ØE+ØØ
.18ØØØØØE+Ø1	.9738347E+ØØ	.9738476E+ØØ
.185ØØØØE+Ø1	.9612612E+ØØ	.9612752E+ØØ
.19ØØØØØE+Ø1	.946285ØE+ØØ	.9463ØØ1E+ØØ
.195ØØØØE+Ø1	.9289435E+ØØ	.9289597E+ØØ
.2ØØØØØØE+Ø1	.9Ø928Ø1E+ØØ	.9Ø92974E+ØØ
.2Ø5ØØØØE+Ø1	.8873439E+ØØ	.8873624E+ØØ
.21ØØØØØE+Ø1	.8631897E+ØØ	.8632Ø93E+ØØ
.215ØØØØE+Ø1	.8368779E+ØØ	.8368987E+ØØ
.22ØØØØØE+Ø1	.8Ø84744E+ØØ	.8Ø84964E+ØØ
.225ØØØØE+Ø1	.778Ø5Ø1E+ØØ	.778Ø732E+ØØ
.23ØØØØØE+Ø1	.745681ØE+ØØ	.7457Ø52E+ØØ
.235ØØØØE+Ø1	.711448ØE+ØØ	.7114732E+ØØ
.24ØØØØØE+Ø1	.6754368E+ØØ	.6754631E+ØØ
.245ØØØØE+Ø1	.6377373E+ØØ	.6377647E+ØØ
.25ØØØØØE+Ø1	.5984437E+ØØ	.5984721E+ØØ

Figure 7: Numerical integration of the differential integral in the text demonstrating the accuracy of the solution compared to the exact value / x y sin(x)

$$y'' + p(x)\,y' + q(x)\,y(x) \;=\; H(x)$$

Let $y' \;=\; z(x)$ so that;

$$z' + p\,z + q\,y \;=\; H$$

Then if $z = u$ and $H - qy - pu = G$

$$\frac{dz}{dx} = G(x, y, u)$$
$$\frac{dy}{dx} = u$$

Using the above transformations the original ode is in a form to be integrated by the Runge-Kutta method.