

## The Laplace Operator- Part 2

In the last Chapter I showed a method for solving a two-dimensional differential equation involving the Laplace operator with boundary conditions. The problem can also be solved numerically using a discrete form of the derivative and Laplacian operators. This chapter ties together some earlier discussion of orthogonal polynomials and matrices. The spectral method linearly expands known and unknown functions with Chebyshev orthogonal polynomials and constants known as the spectrum. The function is known exactly at several grid points identified as collocation points. The collocation points are called Chebyshev-Gauss-Lobatto points. A detailed discussion of the method used to solve 1D and 2D problems is found in Guo <sup>1</sup>.

Most problems solved numerically using collocation methods derive the discrete derivative matrix from a set of rules applied to each element of the matrix (see Binous <sup>2,3</sup>). I will approach the development of this matrix from an integer sequence which is easier to remember and can be applied to any matrix dimension. Consider a second order polynomial in x:

$$[1] \quad P(x) = 2 - (x-1)^2$$

This polynomial when divided by  $(x-1)^2$  is found to be an integer sequence in powers of x

$$[2] \quad P(x)/(x-1)^2 = (2 - (x-1)^2)/(x-1)^2 = 1 + 4x + 6x^2 + 8x^3 + 10x^4 + \dots(2*n+2)x^n$$

where the constant  $(2*n+2)$  applies for all terms with  $n>0$ .

The derivative matrix is formed as an upper triangular matrix with integer sequence in [2] as the off-diagonal elements. The first row, alternates with increasing odd numbers. Each element in the last row is zero. All other rows add 4 to alternating columns to the right. An example of a 11x11 square derivative matrix is:

$$D(Np + 1) = \begin{bmatrix} 0 & 1 & 0 & 3 & 0 & 5 & 0 & 7 & 0 & 9 & 0 \\ 0 & 0 & 4 & 0 & 8 & 0 & 12 & 0 & 16 & 0 & 20 \\ 0 & 0 & 0 & 6 & 0 & 10 & 0 & 14 & 0 & 18 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 & 12 & 0 & 16 & 0 & 20 \\ 0 & 0 & 0 & 0 & 0 & 10 & 0 & 14 & 0 & 18 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 12 & 0 & 16 & 0 & 20 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 14 & 0 & 18 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 20 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 18 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 20 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

It will be shown that this is a similar matrix to the corresponding derivative matrix of Binous. Higher order derivatives can be formed by matrix multiplication. The second derivative matrix is:

$$D^2(Np + 1) = \begin{bmatrix} 0 & 0 & 4 & 0 & 32 & 0 & 108 & 0 & 256 & 0 & 500 \\ 0 & 0 & 0 & 24 & 0 & 120 & 0 & 336 & 0 & 720 & 0 \\ 0 & 0 & 0 & 0 & 48 & 0 & 192 & 0 & 480 & 0 & 960 \\ 0 & 0 & 0 & 0 & 0 & 80 & 0 & 280 & 0 & 648 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 120 & 0 & 384 & 0 & 840 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 168 & 0 & 504 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 224 & 0 & 640 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 288 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 360 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The off-diagonal of the second derivative can be seen to be related to the derivative of equation [2]. Except for the first term all diagonal elements are  $2n*(2n+2)$ . Guo gives an expression for the remaining non-zero terms. If the columns are counted as 0, 1, 2, ...,  $Np$ , then  $Np=10$ . An internal non-zero element (i, j) is calculated as  $j*(j^2-i^2)$ . For example (4, 8) is the coordinate for element  $384 = 8*(64-16)$ . Only the elements in the first row (0, j) are divided by 2.

For one dimensional problems the above derivative matrix can be simplified. For even values of  $Np$  the last  $Np/2+1$  rows can be made zero and last column is made zero. The resulting non-zero entries are in the shape of a "V". I will call this the derivative V matrix. Although it is not a similar matrix to the corresponding derivative matrix of Binous, it can be used for 1D problems involving DV and  $D^2V$  (examples will be shown below).

$$DV(Np + 1) = \begin{bmatrix} 0 & 1 & 0 & 3 & 0 & 5 & 0 & 7 & 0 & 9 & 0 \\ 0 & 0 & 4 & 0 & 8 & 0 & 12 & 0 & 16 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 10 & 0 & 14 & 0 & 18 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 & 12 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 & 0 & 14 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Note: The D matrix can be programmed in Mathematica using the following commands:

```
Temp = IdentityMatrix[Np + 1] - IdentityMatrix[Np + 1]
```

```
Do[Part[Temp, 1, 2 + 2j] = 1 + 2j, {j, 0, Np/2 - 1}]
```

```
Do[Part[Temp, i, Part[Temp, 1, 2 + 2j] + i] = 2 * i + 4j, {i, 2, Np}, {j, 0, Np/2 - Round[i/2]}]
```

```
D = Temp
```

The DV matrix is found by changing line 3 to:

$$\text{Do}[\text{Part}[\text{Temp}, i, \text{Part}[\text{Temp}, 1, 2 + 2j] + i] = 2 * i + 4j, \{i, 2, \text{Np}\}, \{j, 0, \text{Np}/2 - \text{Round}[i - 1/2]\}]$$

$$\text{DV} = \text{Temp}$$

## The Chebyshev Polynomials

In Chapter 23 I showed an expansion of the Chebyshev T polynomial in terms of the Laguerre polynomial. This chapter introduced several other orthogonal polynomials that are solutions to ordinary differential equations. We first show how a known function can be expanded in terms of the Chebyshev T polynomials. Then the Chebyshev polynomial is calculated at several (Np) collocation points and these collocation points are used to derive the spectrum of a known function.

A goal of this chapter for solving a differential equation with boundary conditions is to use the derivative and second derivative matrices defined above with the Chebyshev polynomials and find the spectrum of an **unknown** function. We look for a solution U(z) to the following ODE (g is a positive integer);

$$[3] \quad (1 - z^2) \frac{d^2 U}{dz^2} - 2z \frac{dU}{dz} + g(g + 1)U = 0$$

Let us first consider a known function such as the orthogonal Hermite polynomial. The series of polynomials of increasing degree are represented as H(m, z) where m is the order of the polynomial. We want to express this polynomial as a series of Chebyshev polynomials T(n, z). Let

$$[4] \quad H(m, z) = \sum_{n=0}^{n=\infty} u_n * T(n, z)$$

If we approximate the function at many points, then we can set the upper limit of n to be the number Np. The collocation points z(n) will closely approximate the function H(m, z) and be exactly the value of H(m, z) at the points z(n). Obviously, as Np increases the following series will be a good fit for H(m, z). Define the spectrum u(n) as;

$$[5] \quad u_n = \left( \frac{2}{c(n) * Np} \right) \sum_{p=0}^{p=Np} \left( \frac{1}{c(p)} \right) * T(n, z(p)) * H(m, z(p))$$

Where the functions T and H are evaluated at the Np collocation points z(p) and where c(p) is a constant equal to 2 if n is 0 or Np and equal to 1 otherwise. Then H(m, z(p)) is:

$$[6] \quad H(m, z(p)) = \sum_{n=0}^{n=Np} u_n * T(n, z(p))$$

One reason for using T(n, z(p)) in the expansion is based on a simple relation of the Chebyshev polynomial to the cosine function. Equation [5] is then close to an Fourier expansion but at specific collocation points found in the interval [-1, 1]. Define,

$$[7] \quad z(p) = -\text{Cos}\left[p * \frac{\pi}{Np}\right]$$

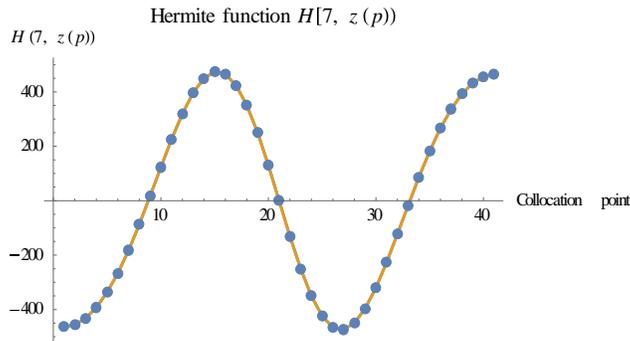
Then it can be shown that

$$[8] \quad T[n, z(p)] = -1^n * \text{Cos}\left[n * p * \frac{\pi}{Np}\right]$$

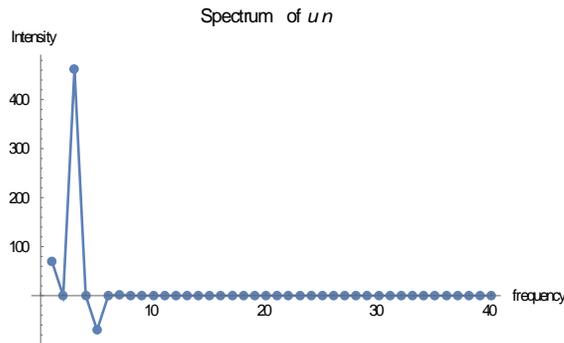
and [6] becomes,

$$[9] \quad H(m, z(p)) = \sum_{n=0}^{n=Np} u_n * (-1)^n * \text{Cos}\left[n * p * \frac{\pi}{Np}\right]$$

The function  $H(7, z(p))$  is shown in the figure below as points  $N_p=40$  over the function  $H(7, z)$ , line:



The spectrum  $u(n)$  of  $H(7, z(p))$  computed from equation [5] is shown below. Note that only odd values of  $n$  below 6 are non-zero intensity. The remaining values are less than  $10^{-16}$ .



The Chebyshev collocation square matrix is developed from equation [8] by varying  $n$  and  $p$  from 0 to  $N_p$ . For  $N_p = 10$  this matrix is,

$$T_{n,p} = \begin{bmatrix} 1.0 & -1.0 & 1.0 & -1.0 & 1.0 & -1.0 & 1.0 & -1.0 & 1.0 & -1.0 & 1.0 \\ 1.0 & -0.951057 & 0.809017 & -0.587785 & 0.309017 & 0. \times 10^{-7} & -0.309017 & 0.587785 & -0.809017 & 0.951057 & -1.0 \\ 1.0 & -0.809017 & 0.309017 & 0.309017 & -0.809017 & 1.0 & -0.809017 & 0.309017 & 0.309017 & -0.809017 & 1.0 \\ 1.0 & -0.587785 & -0.309017 & 0.951057 & -0.809017 & 0. \times 10^{-7} & 0.809017 & -0.951057 & 0.309017 & 0.587785 & -1.0 \\ 1.0 & -0.309017 & -0.809017 & 0.809017 & 0.309017 & -1.0 & 0.309017 & 0.809017 & -0.809017 & -0.309017 & 1.0 \\ 1.0 & 0. \times 10^{-7} & -1.0 & 0. \times 10^{-7} & 1.0 & 0. \times 10^{-7} & -1.0 & 0. \times 10^{-7} & 1.0 & 0. \times 10^{-7} & -1.0 \\ 1.0 & 0.309017 & -0.809017 & -0.809017 & 0.309017 & 1.0 & 0.309017 & -0.809017 & -0.809017 & 0.309017 & 1.0 \\ 1.0 & 0.587785 & -0.309017 & -0.951057 & -0.809017 & 0. \times 10^{-7} & 0.809017 & 0.951057 & 0.309017 & -0.587785 & -1.0 \\ 1.0 & 0.809017 & 0.309017 & -0.309017 & -0.809017 & -1.0 & -0.809017 & -0.309017 & 0.309017 & 0.809017 & 1.0 \\ 1.0 & 0.951057 & 0.809017 & 0.587785 & 0.309017 & 0. \times 10^{-7} & -0.309017 & -0.587785 & -0.809017 & -0.951057 & -1.0 \\ 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \end{bmatrix}$$

Using Mathematica the inverse of this matrix is used to find the derivative matrix using DV(11).

$$[10] \quad Ds(11) = T_{n,p} * DV(11) * T_{p,n}^{-1}$$

$$D_s(11) = \begin{bmatrix} -15.7 & 10.43805 & 8.42492 & -3.92508 & 1.15279 & -0.8 & 0.37508 & -0.14706 & 2.04722 & -5.56591 & 3.7 \\ -12.10472 & 8.25829 & 4.95144 & -1.86376 & 1.35754 & -1.05146 & 0.99361 & -1.53884 & 2.65701 & -3.80423 & 2.14513 \\ -4.65968 & 3.7035 & -1.6 & 1.59405 & 1.82361 & -1.54164 & 2.1764 & -3.44126 & 2.83607 & -0.31464 & -0.5764 \\ 0.4759 & 0.36327 & -4.32015 & 1.94952 & 2.09836 & -1.7013 & 2.60393 & -2.35114 & 0.51592 & 1.73966 & -1.37395 \\ 1.02361 & -0.55387 & -1.3764 & -1.02969 & 1.6 & -1.14164 & 1.63607 & 1.21855 & -2.62361 & 1.50666 & -0.25968 \\ -0.1 & -0.72654 & 2.54164 & -3.07769 & 0.14164 & 0.0 & -0.14164 & 3.07769 & -2.54164 & 0.72654 & 0.1 \\ 0.25968 & -1.50666 & 2.62361 & -1.21855 & -1.63607 & 1.14164 & -1.6 & 1.02969 & 1.3764 & 0.55387 & -1.02361 \\ 1.37395 & -1.73966 & -0.51592 & 2.35114 & -2.60393 & 1.7013 & -2.09836 & -1.94952 & 4.32015 & -0.36327 & -0.4759 \\ 0.5764 & 0.31464 & -2.83607 & 3.44126 & -2.1764 & 1.54164 & -1.82361 & -1.59405 & 1.6 & -3.7035 & 4.65968 \\ -2.14513 & 3.80423 & -2.65701 & 1.53884 & -0.99361 & 1.05146 & -1.35754 & 1.86376 & -4.95144 & -8.25829 & 12.10472 \\ -3.7 & 5.56591 & -2.04722 & 0.14706 & -0.37508 & 0.8 & -1.15279 & 3.92508 & -8.42492 & -10.43805 & 15.7 \end{bmatrix}$$

Using methods for obtaining matrix powers, the second derivative  $D^2$ 's is calculated as  $D_s(11)^2$ .

In matrix notation write [3] as

$$[11] \quad (I - Z^2)D^2U - 2Z * DU + g(g + 1)U = AU = F$$

where  $Z$  is a diagonal matrix of the collocation points  $z(p)$ ,  $I$  is the identity matrix,  $g$  is a given integer and  $F$  is a vector  $\{-\beta, 0, 0, 0, 0, 0, 0, 0, 0, 0, \beta\}^t$ .  $F$  contains two boundary conditions  $[-\beta, \beta]$  and zeros representing the right hand side of the ODE. The symbol  $A$  is a matrix equal to the left side matrix elements of [11]:

$$AU = ((I - Z^2)D^2 - 2Z * D + g(g + 1))U = F$$

where  $A(11)$  is

$$\begin{bmatrix} 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -16.5775 & 23.7936 & 3.3143 & -0.0125 & 2.9616 & -2.4472 & 2.9828 & -5.2236 & 5.9218 & -4.1104 & 1.3972 \\ 5.8799 & -2.3323 & -1.0284 & 7.1601 & 3.8279 & -3.2833 & 5.4082 & -7.0185 & 2.7923 & 5.4739 & -4.8799 \\ 7.4989 & -4.7764 & -3.8627 & 9.7064 & 2.3991 & -1.5528 & 2.3648 & 4.6104 & -8.0816 & 4.0125 & -0.3185 \\ -2.4202 & -0.8324 & 12.7722 & -10.7647 & 9.9284 & 2.0833 & -3.6923 & 11.2231 & -8.0082 & -1.7093 & 3.4202 \\ -2.0 & -1.4472 & 7.7082 & -0.5528 & -5.7082 & 16.0 & -5.7082 & -0.5528 & 7.7082 & -1.4472 & -2.0 \\ 3.4202 & -1.7093 & -8.0082 & 11.2231 & -3.6923 & 2.0833 & 9.9284 & -10.7647 & 12.7722 & -0.8324 & -2.4202 \\ -0.3185 & 4.0125 & -8.0816 & 4.6104 & 2.3648 & -1.5528 & 2.3991 & 9.7064 & -3.8627 & -4.7764 & 7.4989 \\ -4.8799 & 5.4739 & 2.7923 & -7.0185 & 5.4082 & -3.2833 & 3.8279 & 7.1601 & -1.0284 & -2.3323 & 5.8799 \\ 1.3972 & -4.1104 & 5.9218 & -5.2236 & 2.9828 & -2.4472 & 2.9616 & -0.0125 & 3.3143 & 23.7936 & -16.5775 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

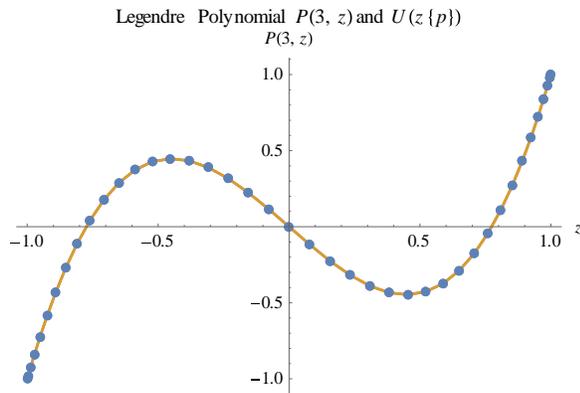
and  $U$  is a solution vector  $\{u_0, u_1, u_2, u_3, u_4, u_5, u_6, u_7, u_8, u_9, u_{10}\}^t$ . Note that rows 1 and 11 in  $A$  have been modified to calculate  $u_0 = -\beta$  and  $u_{10} = \beta$ .

Using  $g = 3$  and  $u_0 = -\beta = -1$  and  $u_{10} = \beta = 1$  the following solution vector  $U$ , is obtained:

$$U = \{-1.0, -0.72401, -0.11025, 0.37399, 0.38976, 0.0, -0.38976, -0.37399, 0.11025, 0.72401, 1.0\}$$

One may have noticed that equation [3] is a differential equation with a known solution<sup>4</sup>. The Legendre Polynomial  $P(3, z)$  (discussed in chapter 23 is the analytical solution to this ODE.

A plot of the solution  $U(z(p))$  versus  $P(3, z)$  is shown with  $N_p = 40$ .



Once the program for expressing an ODE as in equation [11] is written, it is simple to change the number of collocation points and use various values of  $g$  and boundary conditions to find a solution.

## The 2D Laplace Problem

We now use the collocation method to solve the problem posed in Chapter 25. We restate the problem:

Let  $\phi(\xi, \eta) = V(x, y)/V_0$  be the dimensionless potential at coordinates  $(\xi, \eta) = (x/h, y/h)$  and  $V_0$  the potential applied to the cathode. The Laplace potential equation in a plane is:

$$[12] \quad \frac{\partial^2 \phi}{\partial \xi^2} + \frac{\partial^2 \phi}{\partial \eta^2} = 0$$

We assume that the center line  $\eta = 0$ , is at zero potential. Within the electrode region at  $\eta = 1$  the potential is constant. Outside the electrode region the boundary is an insulated/ non-conductor and the perpendicular electric field is zero.

$$[13a, b, c] \quad \begin{aligned} \phi(\xi, 0) &= 0 & \text{all } \xi \\ \phi(\xi, 1) &= 1 & |\xi| \leq L \\ \frac{d\phi(\xi, 1)}{d\eta} &= 0 & |\xi| > L \end{aligned}$$

From symmetry requirements around the center of the electrode at  $\xi = 0$ ,

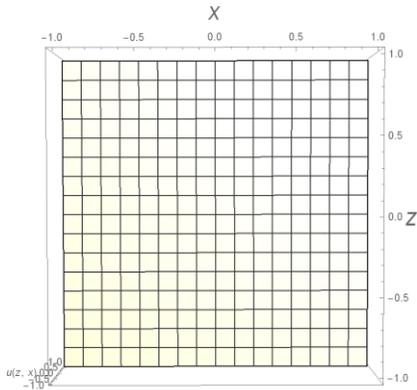
$$[14a, b] \quad \begin{aligned} \frac{d\phi(0, \eta)}{d\xi} &= 0 \\ \frac{d\phi(0, \eta)}{d\eta} &= 1 \end{aligned}$$

These conditions indicate that at the center of the electrode region the field is in a perpendicular direction to the centerline.

Putting the problem in terms of collocation points, two second derivative matrices in the  $\xi$  and  $\eta$  directions are required. If we use  $N_p$  collocation points, then a total of  $(N_p+1) \times (N_p+1)$  points are necessary to define the grid. In addition, we need to consider boundary conditions in two domains requiring the splitting of the  $(N_p+1)^2$  collocation points into two domains. As shown below this leads to



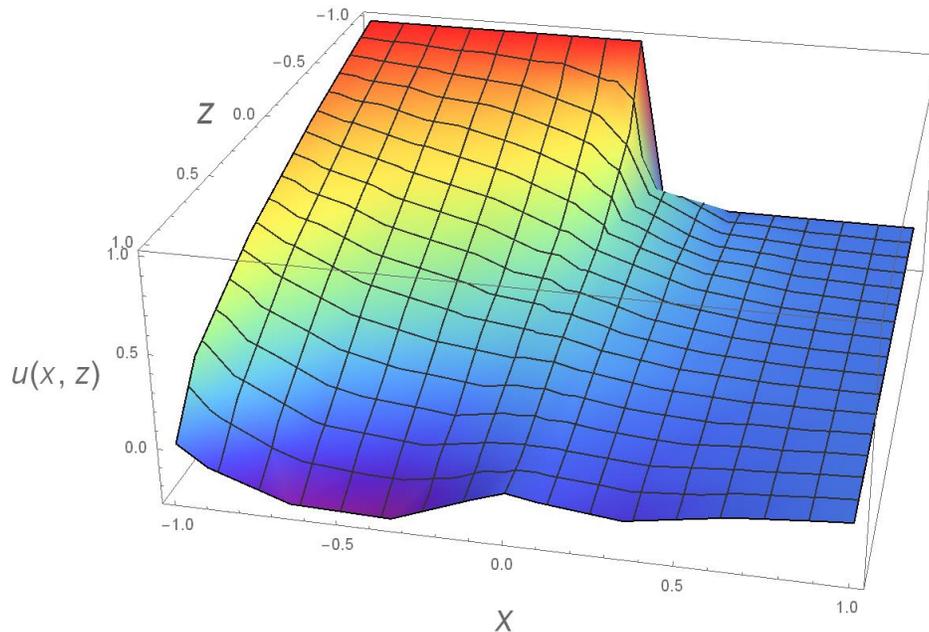
Grid for the 2D Laplacian. In this problem  
 There are 6 vertical and 12 horizontal  
 Collocation points. (not shown)



Since  $U$  and  $F$  have length  $72 = (2 * (N_p + 1))^2$  the  $[36 \times 36]$  matrix  $(D_x^2 + D_z^2)$  needs to be made a  $[72 \times 72]$  matrix. This is required since a solution  $U$  needs to be found in both domains (inside and outside the electrode). This is best accomplished by creating an identity matrix of 72 diagonal elements. The matrices  $(D_x^2 + D_z^2)$  and  $(D_x + D_z)$  are then used to fill in the necessary blocks to match the vectors  $U$  and  $F$ . Several modifications are required to accommodate a continuous solution at the boundary of the two domains by setting  $(D_x + D_z) = 0$  and equating adjacent horizontal collocation points. Boundary conditions such as found in [13c] can be added by letting  $(D_z) = 0$  at the appropriate collocation points when  $z = 1$  and  $x > 0$ . The details of how this matrix is partitioned is explained in Chapter 5 of Guo.

The resulting values of  $U(x, z)$  on the grid are shown in the figure below. The figure shows the correct pattern of potential inside the electrode. Outside the electrode the decay in potential shown to be continuous and the potential extends into the second domain. At the electrode midline there is an unexpected variation in the solution about the boundary conditions of zero potential. It is anticipated that this variation will be reduced by increasing the number of grid points. This is left as a project for the interested student.

Solution to the 2D electrode problem in two domains  
using the Chebyshev Collocation Method



This chapter was added to show that numerical methods are useful to obtain solutions to physical problems in electrodynamics and transport problems involving higher derivatives and dimensions. In principle the numerical method can be applied to higher dimensions and to multiple domains. Mathematical packages are available to handle large matrices and solve systems of linear equations. Effort on the researcher's end is necessary to keep track of variables and develop the appropriate matrices.

Computer numerical methods also allow research in simplifying problems, such as the reduction of derivative matrices as observed in the discovery of the V matrix. We observe that certain ordinary differential equations result in simplified spectral expansions as demonstrated for the Legendre, Hermite and Laguerre differential equations with boundary conditions. In such cases one can compare the numerical results with known analytical solutions.

R Turk  
January 22, 2018

#### References

1. W. Guo, G. Labrosse, R. Narayanan, **The Application of the Chebyshev Spectral Method in Transport Phenomena**, Springer-Verlag, 2012.

2. H. Binous, A. Shaikh, A. Bellagi, *Chebyshev Orthogonal Collocation Technique to Solve Transport Problems with MatLab and Mathematica*, Computer Applications in Engineering Education, Vol. 23(3), Wiley and Sons, 2014.
3. H. Binous, A. Shaikh, A. Bellagi, *Solving Two-dimensional Chemical Engineering Problems using the Chebyshev Orthogonal Collocation Technique*, Computer Applications in Engineering Education, Wiley and Sons, 2016.
4. M. Abramowitz, I. A. Stegun, **Handbook of Mathematical Functions**, Chapter 22, National Bureau of Standards Series 55, 1964.