NUMERICAL METHODS

ECSE 543 - ASSIGNMENT 2

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QUESTION 1

The goal is to find the disjoint local **S**-matrix for each finite element triangle, and subsequently find the global conjoint **S**-matrix for the finite difference mesh composed of the triangular finite elements.

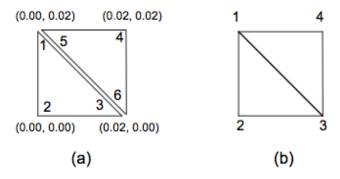


FIGURE 1. a) Disjoint finite elements with local numbering and vertex coordinates (x, y) in meters b) Conjoint finite element mesh with global numbering

The first step to finding the disjoint local **S**-matrix of each finite element triangle is to find the potentials in the elements. We take the potential, U, to vary linearly over the (x, y) plane - note that the assumption of a linearly varying potential within the triangular element is equivalent to assuming that the electric field is uniform within the element (this is a good assumption in parallel-plate conductor type settings). Equation (1) shows the general linear relationship for the potential - constants a, b, and c are to be determined.

$$(1) U = a + bx + cy$$

Date: November 13, 2016.

Denoting the potentials at the vertices by U_v , where v is the vertex number set by the local ordering, we can solve the linear system of equations shown in equation (2) for the constants a, b, and c where the potential at local vertex v has coordinates given by (x_v, y_v) .

(2)
$$\begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} = \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

To solve for the constants we have the closed form relationship shown in equation (3), where adj is used to denote the adjugate of the matrix (found by taking the transpose of its cofactor matrix), and det its determinant.

(3)
$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \frac{adj \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix}}{\det \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix}} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

The result of equation (3) gives us the constants in terms of the vertex potentials as shown in equation (4), where A_e is used to denote the area of the triangular finite element e.

(4)
$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \frac{\begin{bmatrix} (x_2y_3 - x_3y_2) & (x_3y_1 - x_1y_3) & (x_1y_2 - x_2y_1) \\ (y_2 - y_3) & (y_3 - y_1) & (y_1 - y_2) \\ (x_3 - x_2) & (x_1 - x_3) & (x_2 - x_1) \end{bmatrix}}{2A_e} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix}$$

Since the potential in equation (1) can be written as

$$U = \begin{bmatrix} 1 & x & y \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

then we can directly substitute equation (4) into the above representation and rewrite the potential as:

$$U = \sum_{i=1}^{3} \alpha_i(x, y) U_i$$

where the $\alpha_i(x, y)$ (also known as the linear interpolation functions) are given by equations (5), (6), and (7),

(5)
$$\alpha_1 = \frac{1}{2A_e} [(x_2y_3 - x_3y_2) + (y_2 - y_3)x + (x_3 - x_2)y]$$

(6)
$$\alpha_1 = \frac{1}{2A_c} [(x_3y_1 - x_1y_3) + (y_3 - y_1)x + (x_1 - x_3)y]$$

(7)
$$\alpha_1 = \frac{1}{2A_e} [(x_1y_2 - x_2y_1) + (y_1 - y_2)x + (x_2 - x_1)y]$$

and A_e is given by equation (8).

(8)
$$A_e = \frac{1}{2}[(x_2y_3 - x_3y_2) + (x_3y_1 - x_1y_3) + (x_1y_2 - x_2y_1)]$$

The energy in each finite element is given by equation (9), where $W^{(e)}$ is the energy per unit length associated with finite element e, U is the potential - which in general will vary with coordinates (x, y) as was already established, and the integral is swept over A_e , which is the area occupied by element e. *Note that there the permittivity of the medium is neglected in the equation.

$$W^{(e)} = \frac{1}{2} \int_{A_e} |\nabla U|^2 dS$$

Equations (10), and (11) are derived by just making a simple substitution for U in equation (9) using the derived series representation in terms of the interpolation functions and vertex potentials.

(10)
$$W^{(e)} = \frac{1}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} U_i \left[\int_{A_e} \nabla \alpha_i \bullet \nabla \alpha_j dS \right] U_j$$

(11)
$$W^{(e)} = \frac{1}{2} U^T S^{(e)} U$$

Finally we are able to determine the local $S^{(e)}$ depicted in equation (11), whose entries are given by equation (12).

(12)
$$S_{(i,j)}^{(e)} = \int_{A_e} \nabla \alpha_i \bullet \nabla \alpha_j dS$$

Therefore we have:

(13)
$$S_{(1,1)}^{(e)} = \frac{1}{4A} [(y_2 - y_3)^2 + (x_3 - x_2)^2]$$

(14)
$$S_{(1,2)}^{(e)} = \frac{1}{4A}[(y_2 - y_3)(y_3 - y_1) + (x_3 - x_2)(x_1 - x_3)]$$

(15)
$$S_{(1,3)}^{(e)} = \frac{1}{44} [(y_2 - y_3)(y_1 - y_2) + (x_3 - x_2)(x_2 - x_1)]$$

(16)
$$S_{(2,2)}^{(e)} = \frac{1}{4A} [(y_3 - y_1)^2 + (x_1 - x_3)^2]$$

(17)
$$S_{(2,3)}^{(e)} = \frac{1}{44} [(y_3 - y_1)(y_1 - y_2) + (x_1 - x_3)(x_2 - x_1)]$$

(18)
$$S_{(3,3)}^{(e)} = \frac{1}{4A} [(y_1 - y_2)^2 + (x_2 - x_1)^2]$$

(19)
$$S_{(1,2)}^{(e)} = S_{(2,1)}^{(e)}, \quad S_{(3,1)}^{(e)} = S_{(1,3)}^{(e)}, \quad S_{(3,2)}^{(e)} = S_{(2,3)}^{(e)}$$

Letting $S^{(L)}$ represent the disjoint matrix for the lower triangular element in Figure 1.a, and $S^{(U)}$ represent the disjoint matrix for the upper triangular element in Figure 1.b, we can apply some *plug-and-chug* to solve for the matrix entries where the local numberings relative to the derived equations are created in a counterclockwise fashion. The coordinates for the vertices in each element are:

$$\frac{S^{(L)}}{(x1, y1): (0, 00, 0.02)}$$
$$(x2, y2): (0.00, 0.00)$$
$$(x3, y3): (0.02, 0.00)$$

$$\begin{array}{c} S^{(U)} \\ \hline (x1, y1) : & (0.02, 0.02) \\ (x2, y2) : & (0.00, 0.02) \\ (x3, y3) : & (0.02, 0.00) \end{array}$$

We have $A_e = \frac{1}{2}[(0.02 \cdot 0.02)] = 0.0002$, which is identical for e = L and e = U.

$$\begin{split} S_{(1,1)}^{(L)} &= \frac{1}{4(0.0002)}[(0.02)^2] \\ S_{(1,2)}^{(L)} &= \frac{1}{4(0.0002)}[(0.02)(-0.02)] \\ S_{(1,3)}^{(L)} &= \frac{1}{4(0.0002)}[0] \\ S_{(2,2)}^{(L)} &= \frac{1}{4(0.0002)}[(-0.02)^2 + (-0.02)^2] \\ S_{(2,3)}^{(L)} &= \frac{1}{4(0.0002)}[(-0.02)(0.02)] \\ S_{(3,3)}^{(L)} &= \frac{1}{4(0.0002)}[(0.02)^2] \\ S_{(1,2)}^{(L)} &= S_{(2,1)}^{(L)}, \quad S_{(3,1)}^{(L)} &= S_{(1,3)}^{(L)}, \quad S_{(3,2)}^{(L)} &= S_{(2,3)}^{(L)} \\ S_{(1,2)}^{(L)} &= \begin{bmatrix} 0.5 & -0.5 & 0 \\ -0.5 & 1 & -0.5 \\ 0 & -0.5 & 0.5 \end{bmatrix} \\ \end{split}$$

$$\begin{split} S_{(1,1)}^{(U)} &= \frac{1}{4(0.0002)}[(0.02)^2 + (0.02)^2] \\ S_{(1,2)}^{(U)} &= \frac{1}{4(0.0002)}[(0.02)(-0.02)] \\ S_{(1,3)}^{(U)} &= \frac{1}{4(0.0002)}[(0.02)(-0.02)] \\ S_{(2,2)}^{(U)} &= \frac{1}{4(0.0002)}[(-0.02)^2] \\ S_{(2,3)}^{(U)} &= \frac{1}{4(0.0002)}[0] \\ S_{(3,3)}^{(U)} &= \frac{1}{4(0.0002)}[(-0.02)^2] \\ S_{(1,2)}^{(U)} &= S_{(2,1)}^{(U)}, \quad S_{(3,1)}^{(U)} &= S_{(1,3)}^{(U)}, \quad S_{(3,2)}^{(U)} &= S_{(2,3)}^{U} \\ S_{(1,2)}^{(U)} &= \begin{bmatrix} 1 & -0.5 & -0.5 \\ -0.5 & 0.5 & 0 \\ -0.5 & 0 & 0.5 \end{bmatrix} \\ \end{split}$$

The global conjoint S-matrix can be found using the disjoint finite element $S^{(e)}$ matrices. The energy of the entire finite element mesh is found by summing the energies of each individual element as is shown in equation (20).

(20)
$$W = \sum_{L,U} W^{(e)} = \frac{1}{2} U_{dis}^T S_{dis} U_{dis}$$

where

$$S_{dis} = \begin{bmatrix} S^{(L)} \\ S^{(U)} \end{bmatrix} = \begin{bmatrix} 0.5 & -0.5 & 0 & 0 & 0 & 0 \\ -0.5 & 1 & -0.5 & 0 & 0 & 0 \\ 0 & -0.5 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -0.5 & -0.5 \\ 0 & 0 & 0 & -0.5 & 0.5 & 0 \\ 0 & 0 & 0 & -0.5 & 0 & 0.5 \end{bmatrix}$$

Substituting $U_{dis} = CU_{con}$ (whose relationship is shown in equation (21)) into equation (20), gives

$$W = \frac{1}{2} U_{con}^T C^T S_{dis} C U_{con}$$

where $S = C^T S_{dis} C$

$$\begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \\ U_5 \\ U_6 \end{bmatrix}_{dis} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{bmatrix}_{conj}$$

therefore

$$C = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Carrying out the matrix multiplication we have the following for the global S-matrix (which was computed using MATLAB).

FIGURE 2. MATLAB computation of the global S-matrix

$$S = \begin{bmatrix} 1 & -0.5 & 0 & -0.5 \\ -0.5 & 1 & -0.5 & 0 \\ 0 & -0.5 & 1 & -0.5 \\ -0.5 & 0 & -0.5 & 1 \end{bmatrix}$$

QUESTION 2

Part a. Using the two-element mesh shown in Figure 1 as a building block, a finite element mesh is constructed for one-quarter of the cross-section of the coaxial cable shown in Figure 3. The equivalent one-quarter mesh is shown in Figure 4. To simplify the node coordinates in subsequent calculations, the x, y coordinates were renormalized to the bottom left corner of Figure 4.

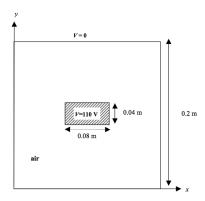


FIGURE 3. Rectangular coax.

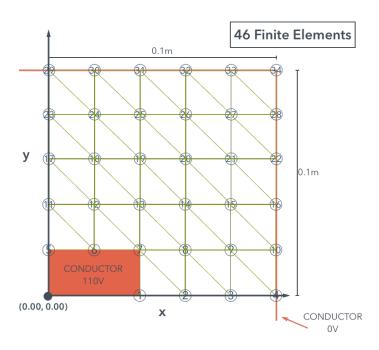


FIGURE 4. Global ordering of a finite element mesh for one quarter of a coax.

node.dat			bc.dat			tri.da	ţ		
1	0.04	0.00	5	110	0.0	1	2	7	0
2	0.06	0.00	6	110	0.0	2	8	7	0
3	0.08	0.00	7		0.0	2	3	8	0
4	0.10	0.00	4	0.		3	9	8	0
5	0.00	0.02	10		.0	3	4	9	0
6	0.02	0.02	16		.0	4	10	9	0
7	0.04	0.02	22	0.		5	6	11	0
8	0.06	0.02	28		.0	6	12	11	0
9	0.08	0.02	34		.0	6	7	12	0
10	0.10	0.02	33		.0	7	13	12	0
11	0.00	0.04	32		.0	7	8	12	0
12	0.02	0.04	31		.0	8	14	13	0
13	0.04	0.04	30		.0	8	9	14	0
14	0.06	0.04	29	0.	.0	9	15	14	0
15 16	$0.08 \\ 0.10$	$0.04 \\ 0.04$				9 10	10 16	15 15	0
17	0.10	0.04 0.06				10	12	17	0
18	0.00	0.06				12	18	17	0
19	0.02	0.06				12	13	18	0
20	0.04	0.06				13	19	18	0
21	0.08	0.06				13	14	19	0
22	0.10	0.06				14	20	19	0
23	0.00	0.08				14	15	20	0
$\frac{1}{24}$	0.02	0.08				15	21	20	0
25	0.04	0.08				15	16	21	0
26	0.06	0.08				16	22	21	0
27	0.08	0.08				17	18	23	0
28	0.10	0.08				18	24	23	0
29	0.00	0.10				18	19	24	0
30	0.02	0.10				19	25	24	0
31	0.04	0.10				19	20	25	0
32	0.06	0.10				20	26	25	0
33	0.08	0.10				20	21	26	0
34	0.10	0.10				21	27	26	0
						21	22	27	0
						22	28	27	0
						23	24	29	0
						24	30	29	0
						24	25	30	0
						25	30	31	0
						25	26	31	0
						26	32	31	0
						26	27	32	0
						27	33	32	0
						27	28	33	0
_	D		MADI DOD	c		28	34	33	0

TABLE 1. SIMPLE2D input consisting of node coordinates, boundary conditions, and finite element vertex definitions from left to right

The input file used for the SIMPLE2D Matlab program was split up into three files, *node.dat*, *bc.dat*, *tri.dat*, which are shown in Table 1. The *node.dat* table lists the node numbers (according to the global ordering shown in Figure 4) and their respective x, y coordinates; the *bc.dat* file lists the boundary nodes

(according to the global ordering), and their respective potentials in Volts; lastly the *tri.dat* table lists the nodes (according to the global ordering) that make up each triangular finite element with a zero terminated column. The data was split up for convenience of comprehension, however could've just as easily been stacked in a single file.

Part b. The electrostatic potential solution was computed using the SIMPLE2D program with the mesh shown in Table 1. The screenshot from the Matlab output is shown in Figure 5 - note that the coordinates shown in the Matlab output correspond to the renormalized x, y problem coordinates. From the output, we deduce that by symmetry of the problem, the potential at point (0.06, 0.04) is equivalent to the potential at node 19 in Figure 4. The potential at (0.06, 0.04) is 41.4710 Volts.

С	ommand Windo	ow			
	>> potential	s = SIMPLE	2D_M('nod	e.dat', 'tri.dat	', 'bc.dat')
	potentials =	:			
	1.0000	0.0400	0	88.0136	
	2.0000	0.0600	0	66.0271	
	3.0000	0.0800	0	32.5085	
	4.0000	0.1000	0	0	
	5.0000	0	0.0200	110.0000	
	6.0000	0.0200	0.0200	110.0000	
	7.0000	0.0400	0.0200	110.0000	
	8.0000	0.0600	0.0200	71.7932	
	9.0000	0.0800	0.0200	32.0035	
	10.0000	0.1000	0.0200	0	
	11.0000	0	0.0400	83.2537	
	12.0000	0.0200	0.0400	85.2655	
	13.0000	0.0400	0.0400	65.5451	
	14.0000	0.0600	0.0400	47.6714	
	15.0000	0.0800	0.0400	23.7123	
	16.0000	0.1000	0.0400	0	
	17.0000	0	0.0600	52.4836	
	18.0000	0.0200	0.0600	50.7925	
	19.0000	0.0400	0.0600	41.4710	
	20.0000	0.0600	0.0600	29.6352	
	21.0000	0.0800	0.0600	15.1743	
	22.0000	0.1000	0.0600	0	
	23.0000	0	0.0800	25.0959	
	24.0000	0.0200	0.0800	23.9499	
	25.0000	0.0400	0.0800	19.9112	
	26.0000	0.0600	0.0800	14.2240	
	27.0000	0.0800	0.0800	7.3496	
	28.0000	0.1000	0.0800	0	
	29.0000	0	0.1000	0	
	30.0000	0.0200	0.1000	0	
	31.0000	0.0400	0.1000	0	
	32.0000	0.0600	0.1000	0	
	33.0000	0.0800	0.1000	0	
	34.0000	0.1000	0.1000	0	

FIGURE 5. SIMPLE2D Matlab output for the quarter-coax finite element mesh with renormalized x, y coordinates.

Part c. To compute the capacitance per unit length obtained from the solution of the SIMPLE2D program, we start off by finding the energy per unit length contained in a square made up of two triangular finite elements:

$$W = \frac{1}{2} \epsilon_0 U_{con}^T S U_{con}$$

where the global S matrix is that found in Question 1, and U_{con} represents the vector of conjoint potentials according to the global ordering. After finding the energy in every micro-grid of the free-node problem domain (**not including the fixed potential domain**). We then sum up all of those energies, and multiply by 4 to obtain the energy per unit length in the entire free-space of the coax $W^{(total)} = 4 * \sum_{q} W$. We then use

$$W^{(total)} = \frac{1}{2}CV^2$$

where C is the capacitance per unit length, and V is the potential difference across the coax (V = 110 Volts - 0 Volts in this case). The Matlab script used to carry out the above procedure is shown in Listing 1 - again this Matlab script is based on the specific global ordering of Figure 4.

```
clear all;
  potentials = SIMPLE2D_M('node.dat', 'tri.dat', 'bc.dat')
  S = [1.0000]
                  -0.5000
                                         -0.5000
       -0.5000
                   1.0000
                              -0.5000
                  -0.5000
                              1.0000
                                         -0.5000
       -0.5000
                         0
                              -0.5000
                                          1.0000];
  permittivity = 8.85418782e - 12;
  const = 0.5 * permittivity;
13 boundary = [4,10,16,22,28,34];
  W = 0;
15
  for i = 1:28
17
       if any(i == boundary)
19
           continue
       end
       v = [i, i+1, i+7, i+6];
       all_U = potentials(:,4);
23
       U = [\,all_-U\,(v\,(1));\ all_-U\,(v\,(2));\ all_-U\,(v\,(3));\ all_-U\,(v\,(4))];
      W = W + (U' * S * U);
27 end
29 | W = W .* const;
|C| = 4*W / (0.5 * (110^2))
```

LISTING 1. capacitance_pul.m

The capacitance per unit length is: 5.2627e - 11 Farads/m

QUESTION 3

The conjugate gradient method implementation provided in Listing 4 is used to construct the finite difference equation for a quadrant of the coax, and subsequently solve it. The output for h=0.02 is shown in Figure 8. Note that the value for h is inputed by the user in the conjugate gradient program, thereby making it very easy to simply try out the problem with different inter-element spacings.

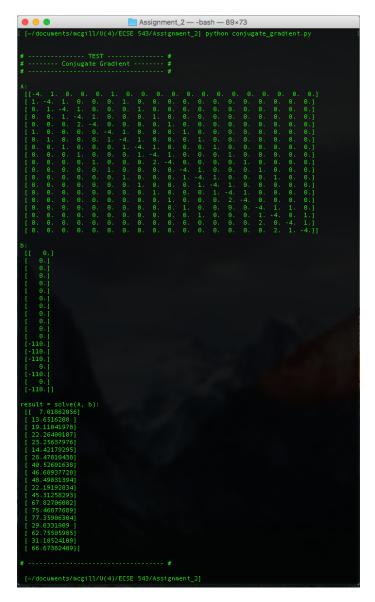


FIGURE 6. Console output of conjugate gradient solver used to solve the unpreconditioned finite difference equation of the bottom-left quadrant of the coax

Part a. The finite difference matrix is tested using the choleski decomposition program written for Question 1 of Assignment 1 to ensure that it is positive definite. The choleski decomposition implementation is provided in Listing 5 again for convenience. The console output is provided in Figure 7. Unfortunately as it is, the matrix is NOT positive definite. To make it positive definite, we could precondition the finite difference system of equations with the transpose of the matrix. In other words instead of solving Ax = b, we could solve HAx = Hb where $H = A^T$.

FIGURE 7. Console output of choleski solver used to solve the unpreconditioned finite difference equation of the bottom-left quadrant of the coax

Part b. The modified preconditioned problem is solved using the conjugate gradient method, and the choleski decomposition method. The console outputs are shown in Figures 8 and 9.



FIGURE 8. Console output of conjugate graident solver used to solve the preconditioned finite difference equation of the bottom-left quadrant of the coax

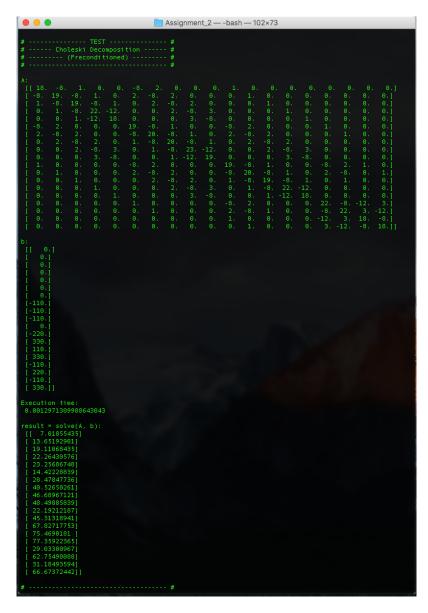


FIGURE 9. Console output of choleski solver used to solve the preconditioned finite difference equation of the bottom-left quadrant of the coax

Part c. A plot of the 2-norm and the infinity-norm of the residual versus iterations for the conjugate gradient program is shown below in Figure 10.

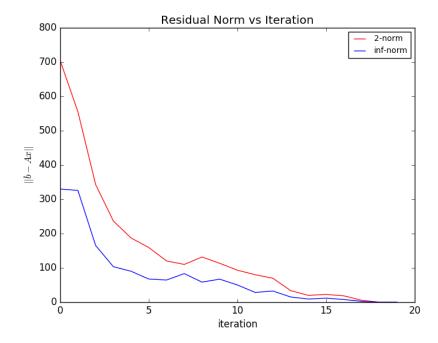


FIGURE 10. Plot of the 2-norm and the infinity-norm of the residual versus iterations for the conjugate gradient program.

Part d. The potential at (x,y) = (0.06, 0.04) is 40.52601638 Volts using the conjugate gradient method, and 40.52650261 Volts using the choleski decomposition method. The corresponding console outputs are shown in Figures 11 and 12. These results are very similar to the potential computed in Question 2(b), which as we recall was found to be 41.4710 Volts. It is interesting to note that the potentials computed using conjugate gradient and choleski appears to be more accurate than that found using the SIMPLE2D program in Question 2(b). The potentials found also are very similar to the potential found at the same (x,y) location and for the same node spacing computed in Assignment 1 using SOR - which was found to be 40.5265 Volts on aggregate spanning over the multiple different values for the parameter ω . This seems to indicate that the methods that use the finite difference method all perform similarly, and perhaps more accurately than the finite element method when the finite elements are distributed as they are in Figure 4.

```
Assignment_2 — -bash — 119×73
                        ------ TEST ------
Conjugate Gradient -
result = solve(A, b):

[[ 7.01862056]

[ 13.6516208 ]

[ 19.11041978]

[ 22.26400107]

[ 23.25637976]

[ 14.42179295]
   tential (0.06,
40.52601638]
```

FIGURE 11. Console output computing the potential at (0.06, 0.04) using the conjugate gradient method

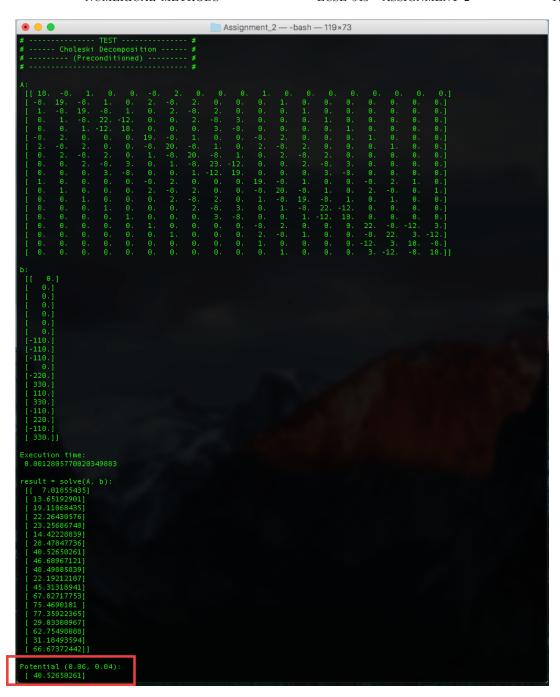


FIGURE 12. Console output computing the potential at (0.06, 0.04) using the choleski decomposition method

Part e. To compute the capacitance per unit length of the system from the finite difference solution, one could use a finite element energy equation, where the vertices of the finite elements are the nodes in the finite difference mesh. Since these potentials are known, the corresponding energies per unit length of each free potential finite element can also be determined. The energies of the individual finite elements can be subsequently added, and then one can simply used the capacitance energy equation from Question 2 to determine the capacitance per unit length of the system. Thus we have computed the capacitance per unit length from the finite difference solution.

```
#
  # Experiment
  # Author: Mido Assran
5 # Date: Nov. 10, 2016
  # Description: Experiment solves the finite difference equations using
7 # both the ConjugateGradientFiniteDifferencePotentialSolver and the
 # CholeskiDecomposition solver, and performs postprocessing to
9 # plot and compare the results.
11 import numpy as np
  import matplotlib.pyplot as plt
13 from utils import matrix_dot_matrix, matrix_transpose
  from conjugate_gradient import ConjugateGradientFiniteDifferencePotentialSolver
15 from choleski import Choleski Decomposition
17 if __name__ == "__main__":
     print("\n", end="\n")
     19
     print ("# ----- Conjugate Gradient ----- #", end="\n")
     21
     cgfdps = ConjugateGradientFiniteDifferencePotentialSolver(h=0.02)
     A = matrix_dot_matrix(matrix_transpose(cgfdps._A), cgfdps._A)
23
     b = matrix_dot_matrix(matrix_transpose(cgfdps._A), cgfdps._b)
25
     cgfdps.A = A; cgfdps.b = b
     potential_history, residual_history, search_history = cgfdps.solve()
     print ("A:\n", cgfdps._A, end="\n\n")
27
     print ("b:\n", cgfdps._b, end="\n\n")
     print("result = solve(A, b): \n", potential_history[-1], end="\n\n")
29
     node_number = cgfdps.map_coordinates_to_node((0.06, 0.04))
31
     potential = potential_history[-1][node_number]
     print ("Potential (0.06, 0.04):\n", potential, end="\n\n")
33
     35
     print("\n", end="\n")
     print ("# — #", end="\n")
print ("# — #", end="\n")
37
```

```
print("# -----
                                                   39
       chol_d = CholeskiDecomposition()
       A = cgfdps.A
41
       b = cgfdps._b
43
       print("A: \n", A, end="\n\n")
       print ("b:\n", b, end="\n\n")
45
       v = chol_d.solve(A=A, b=b)
       \mathbf{print}("\,result\,=\,solve\,(A,\,\,b\,)\colon \backslash\, n"\,,\,\,\mathbf{v}\,,\,\,\mathbf{end}\!\!=\!"\,\backslash\, n\,\backslash\, n"\,)
47
       49
       print("\n", end="\n")
51

      print ( \n , end= \n )
      #", end="\n")

      print ("# — Choleski Decomposition — #", end="\n")

      print ("# — (Preconditioned) — #", end="\n")

      print ("# — #", end="\n")

      abol d — Choleski Decomposition ()

53
55
       chol_d = CholeskiDecomposition()
       # Create a symmetric, real, positive definite matrix.
       A = matrix_dot_matrix(matrix_transpose(cgfdps._A), cgfdps._A)
       b = matrix_dot_matrix(matrix_transpose(cgfdps._A), cgfdps._b)
59
       print("A: \n", A, end="\n\n")
61
       print("b:\n", b, end="\n\n")
       v = chol_d.solve(A=A, b=b)
63
       print ("result = solve (A, b):\n", v, end="\n")
65
       node_number = cgfdps.map_coordinates_to_node((0.06, 0.04))
       potential = v[node_number]
67
       print ("Potential (0.06, 0.04):\n", potential, end="\n\n")
       69
71
       # Perform postprocessing of ConjugateGradient residual history
       fig , ax = plt.subplots()
73
       norm_2 = [np.linalg.norm(v) for i, v in enumerate(residual_history)]
       norm_inf = [np.linalg.norm(v, np.inf) for i, v in enumerate(residual_history)]
75
       ax.plot(norm_2, 'r', label="2-norm")
       ax.plot(norm_inf, 'b', label="inf-norm")
77
```

```
legend = ax.legend(loc='best', fontsize='small')
       plt.title('Residual Norm vs Iteration')
79
       plt.ylabel(r'$||b - Ax||$')
plt.xlabel('iteration')
81
       plt.show()
```

LISTING 2. experiment.py

```
2 # Utils
4 # Author: Mido Assran
  # Date: 5, October, 2016
6 # Description: Utils provides a cornucopia of useful matrix
  # and vector helper functions.
  import random
10 import numpy as np
12 def matrix_transpose(A):
      :type A: np.array([float])
14
       :rtype: np.array([floats])
16
      # Initialize A_T(ranspose)
18
      A_T = \text{np.empty}([A. \text{shape}[1], A. \text{shape}[0]])
20
      # Set the rows of A to be the columns of A_T
       for i, row in enumerate(A):
22
           A_T[:, i] = row
24
       return A<sub>-</sub>T
26
  def matrix_dot_matrix(A, B):
28
       :type A: np.array([float])
30
       :type B: np.array([float])
       :rtype: np.array([float])
32
34
      # If matrix shapes are not compatible return None
       if (A. shape [1] != B. shape [0]):
36
           return None
38
```

```
A_{dot_B} = np.empty([A.shape[0], B.shape[1]])
      A_{dot_B}[:] = 0 # Initialize entries of the new matrix to zero
40
      B_T = matrix_transpose(B)
42
      for i, row_A in enumerate(A):
44
           for j, column_B in enumerate(B_T):
               for k, v in enumerate(row_A):
46
                   A_{dot_B}[i, j] += v * column_B[k]
48
      return A_dot_B
50
52 def matrix_dot_vector(A, b):
      :type A: np.array([float])
54
      :type b: np.array([float])
      :rtype: np.array([float])
56
58
      # If matrix shapes are not compatible return None
      if (A. shape [1] != b. shape [0]):
60
           return None
62
      A_{dot_b} = np.empty([A.shape[0]])
      A_{-}dot_{-}b[:] = 0 # Initialize entries of the new vector to zero
64
      for i, row_A in enumerate(A):
66
           for j, val_b in enumerate(b):
               A_dot_b[i] += row_A[j] * val_b
68
      return A_dot_b
70
72
  def vector_to_diag(b):
74
      :type b: np.array([float])
      :rtype: np.array([float])
76
```

```
78
       diag_b = np.empty([b.shape[0], b.shape[0]])
       \operatorname{diag_-b}[:] = 0
                          # Initialize the entries to zero
80
       for i, val in enumerate(b):
82
           diag_b[i, i] = val
84
       return diag_b
86
   def generate_positive_semidef(order, seed=0):
88
       :type order: int
       :type seed: int
90
       :rtype: np.array([float])
92
       np.random.seed(seed)
94
       A = np.random.randn(order, order)
96
       A = matrix_dot_matrix(A, matrix_transpose(A))
       # TODO: Replace matrix_rank with a custom function
98
       from numpy.linalg import matrix_rank
       if matrix_rank(A) != order:
100
           print("WARNING: Matrix is singular!", end="\n\n")
102
       return A
```

LISTING 3. utils.py

```
# Conjugate Gradient Finite Difference Potential Solver
  # Author: Mido Assran
5 # Date: Nov. 10, 2016
  # Description: ConjugateGradientFiniteDifferencePotentialSolver determines
7 # the electric potential at all vertices in a finite element mesh
  # of a coax.
9
  import random
11 import numpy as np
  from conductor_description import *
13 from utils import matrix_dot_matrix, matrix_transpose
15 import warnings
  warnings.filterwarnings("ignore", category=np.VisibleDeprecationWarning)
17
  DEBUG = False
19
  class ConjugateGradientFiniteDifferencePotentialSolver(object):
21
      " " "
      :-----Instance Variables ----:
23
      :type _h: float -> The inter-mesh node spacing
25
      :type _num_x_points: float -> Number of mesh points in the x direction
      :type _num_y_points: float -> Number of mesh points in the y direction
      :type _potentials: np.array([float]) -> Electric potential at nodes
27
29
      def __init__(self, h=0.02):
31
          :type h: float
          :rtype: void
33
35
          np.core.arrayprint._line_width = 200
37
          self._h = h
```

```
39
           self._conductor_indices = \
               self.map_coordinates_to_indices((INNER_COORDINATES[0],INNER_COORDINATES[1]))
41
           self._conductor_index_dimensions = \
               (INNER\_HALF\_DIMENSIONS[0] / self.\_h + 1, INNER\_HALF\_DIMENSIONS[1] / self.\_h + 1)
43
          # Create the finite difference system of linear equations
45
           self._A, self._b = self.create_fdm_equation()
47
           if DEBUG:
               print (self._A, "\n^n, self._b)
49
51
      # Helper function converts node indices to locations in the mesh
      def map_indices_to_coordinates(self, indices):
53
           :type indices: (int, int)
55
           :rtype: (float, float)
57
          h = self.h
59
          return (indices [0] * h , indices [1] * h)
61
      # Helper function that converts node locations in the mesh to indices
63
      def map_coordinates_to_indices(self, coordinates):
65
           :type coordinates: (float, float)
          :rtype: (int, int)
67
          h = self.h
69
71
          i, j = 0, 0
          x, v = 0, 0
73
          while (coordinates [0] - x) > (0.5 * h):
              x += h
75
               i += 1
77
```

```
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```

```
while (coordinates [1] - y) > (0.5 * h):
               y += h
79
               j += 1
81
           indices = (i, j)
           return indices
83
85
       def create_fd_grid(self):
87
           :rtype: np.array([float, float])
89
           h = self.h
91
           x_midpoint = INNER_COORDINATES[0] + INNER_HALF_DIMENSIONS[0]
           y_midpoint = INNER_COORDINATES[1] + INNER_HALF_DIMENSIONS[1]
93
           num_x_points = int(x_midpoint / h + 1)
           num_y_points = int(y_midpoint / h + 1)
95
           num_nodes = num_x_points * num_y_points
97
           # Initialize potentials matrix according to the boundary coniditions
           grid = np.empty((num_x_points, num_y_points))
99
           grid[:] = 0
101
           return grid
103
       def create_free_potentials_vector(self, fd_grid):
105
           :type fd_grid: np.array([float, float])
           :rtype: (np.array([float]), list((int, int)))
107
           h = self._h
109
           fp_map = []
111
           fpv = []
113
           y_i = 0
115
           while y_i < fd_grid.shape[1]:
               for x_i, _ in enumerate(fd_grid[:, y_i]):
```

```
coordinates = self.map_indices_to_coordinates((x_i, y_i))
117
                    # If not in a fixed potential conductor add to free vector
119
                    if (not ((coordinates [0] >= INNER_COORDINATES [0])
                            and (coordinates [1] >= INNER_COORDINATES [1]))
121
                        and not (coordinates [0] = 0 or coordinates [1] = 0):
                        fpv.append(0)
123
                        fp_map.append((x_i, y_i))
                y_i += 1
125
            fpv = np.array(fpv)
127
            return (fpv, fp_map)
129
       def map_node_to_indices(self, node_number):
131
            :type node_number: int
133
            :rtype: (int, int)
135
            return self.fp_map[node_number]
137
       def map_coordinates_to_node(self, coordinates):
            indices = self.map_coordinates_to_indices(coordinates)
139
            return self.map_indices_to_node(indices)
141
       def map_indices_to_node(self, indices):
143
           :type indices: (int, int)
145
            :rtvpe: int
            for i, v in enumerate (self.fp_map):
147
                if v == indices:
149
                    return i
            return None
151
       def create_fd_equation_matrices(self, fd_grid, num_free_potentials):
153
            :type fd_grid: np.array([float, float])
            :type num_free_potentials: float
155
```

```
:rtype: (np.array([float, float]), np.array([float]))
157
           w_c, h_c = self._conductor_index_dimensions
159
           i_c, j_c = self.\_conductor\_indices
           num_x_points, num_y_points = fd_grid.shape
161
           A = np.empty([num_free_potentials, num_free_potentials])
           A[:] = 0.0
163
           b = np.empty([num_free_potentials])
           b[:] = 0.0
165
           for ref_p in range(num_free_potentials):
167
               A[ref_p, ref_p] = -4.0
169
               # Apply boundary conditions
171
               i, j = self.map_node_to_indices(ref_p)
173
               # Determine adjacent node numbers
               left_p = ref_p - 1
175
                right_p = ref_p + 1
                top_p = ref_p + (num_x_points - 1)
177
                bottom_p = ref_p - (num_x_points -1)
179
                if (j >= j_c):
                    top_p = ref_p + (num_xpoints - 1 - w_c)
                if (j = num_ypoints - 1):
181
                    bottom_p = ref_p - (num_x_points - 1 - w_c)
183
               # These might fail at the boundaries
185
                trv:
                   A[ref_p, top_p] = 1.0
187
                except:
189
                    pass
                try:
                    if bottom_p >= 0:
191
                        A[ref_p, bottom_p] = 1.0
193
                except:
                    pass
```

```
195
                try:
                    A[ref_p, right_p] = 1.0
                except:
197
                    pass
199
                try:
                    if left_p >= 0:
                        A[ref_p, left_p] = 1.0
201
                except:
203
                    pass
               # Apply boundary conditions
205
                if (i = num_x-points - 1):
207
                    # Apply neumann boundary conditions to A
                    A[ref_p, left_p] += 1.0
                    trv:
209
                        A[ref_p, right_p] = 0.0
                    except:
211
                        pass
                if (i = 1):
213
                    # Apply dirichlet boundary conditions to b
215
                    b[ref_p] = 0
                    try:
                        A[ref_p, left_p] = 0.0
217
                    except:
                        pass
219
                if (i == i_c - 1) and (j >= j_c):
                    # Apply dirichlet boundary conditions to b
221
                    b[ref_p] -= CONDUCTOR_POTENTIAL
                    try:
223
                        A[ref_p, right_p] = 0.0
                    except:
225
                        pass
227
                if (i >= i_c) and (j == j_c - 1):
                    # Apply dirichlet boundary conditions to b
229
                    b [ref_p] -= CONDUCTOR_POTENTIAL
                    try:
                        A[ref_p, top_p] = 0.0
231
                    except:
233
                        pass
```

```
A[ref_p, bottom_p] += 1.0
237
                        A[ref_p, top_p] = 0.0
                    except:
239
                        pass
                if (j == 1):
241
                    # Apply dirichlet boundary conditions to b
                    b[ref_p] = 0.0
243
                    try:
245
                        A[ref_p, bottom_p] = 0.0
                    except:
247
                        pass
           b = b.reshape(b.shape[0], 1)
249
            return A, b
251
253
       def create_fdm_equation(self):
            :rtype: (np.array([float, float]), np.array([float]))
255
257
            self.fd_grid = self.create_fd_grid()
            self.fp_v, self.fp_map = self.create_free_potentials_vector(self.fd_grid)
           A, b = self.create_fd_equation_matrices(fd_grid=self.fd_grid,
259
                                                    num_free_potentials=len(self.fp_v)
261
            return A, b
263
       def solve(self):
265
            :rtype: [np.array([float]), np.array([float]), np.array([float])]
267
269
           A = self.A
           b = self._b
271
            num_eigenvalues = A. shape [1]
```

if $(j = num_ypoints - 1)$:

235

Apply neumann bondary conditions to A

```
273
           # Potentials
           x_h = []
275
           x = np.empty([A.shape[1], 1])
           x[:] = 0
277
           x_h. append (x)
279
           # Residuals
           r_h = []
281
            r = b - matrix_dot_matrix(A, x)
            r_h. append (r)
283
           # Search direction
285
            p_h = []
           p = r
287
            p_h. append (p)
289
            for k in range(num_eigenvalues):
291
                # Linear search
293
                alpha = (matrix_dot_matrix(matrix_transpose(p), r)
                         / matrix_dot_matrix (matrix_dot_matrix (matrix_transpose(p), A), p)
                         [0,0]
295
                x = x + alpha * p
297
                # Find new search direction
                r = b - matrix_dot_matrix(A, x)
299
                beta = -1.0 * (matrix_dot_matrix(matrix_dot_matrix(matrix_transpose(p), A), r)
                        / matrix_dot_matrix(matrix_dot_matrix(matrix_transpose(p), A), p)
301
                         [0,0]
                p = r + beta * p
303
305
                # Log history
                x_h. append (x)
307
                r_h. append (r)
                p_h. append (p)
309
            return (x_h, r_h, p_h)
311
```

```
if __name__ == '__main__':
         print("\n", end="\n")

      print ("# ______ TEST ______ #", end="\n")

      print ("# _____ Conjugate Gradient _____ #", end="\n")

      print ("# ______ tend="\n")

      #", end="\n")

      #", end="\n")

315
          cgfdps = ConjugateGradientFiniteDifferencePotentialSolver(h=0.02)
317
          potential_history, residual_history, search_history = cgfdps.solve()
          print("A: \n", cgfdps.\_A, end="\n\n")
319
          print("b:\n", cgfdps.b, end="\n\n")
         print("result = solve(A, b): \n", potential_history[-1], end="\n'")
321
                                                     #", end="\n\n")
          print ("# ----
```

LISTING 4. conjugate_gradient.py

```
2 # Choleski Decomposition
4 # Author: Mido Assran
  # Date: 30, September, 2016
6 # Description: CholeskiDecomposition solves the linear system of equations:
  # Ax = b by decomposing matrix A using Choleski factorization and using
8 # forward and backward substitution to determine x. Matrix A must
  # be symmetric, real, and positive definite.
10
  import random
12 import timeit
  import numpy as np
14 from utils import matrix_transpose
16 DEBUG = True
18 class CholeskiDecomposition (object):
20
      def __init__(self):
           if DEBUG:
              np.core.arrayprint._line_width = 200
22
      def solve (self, A, b, band=None):
24
           :type A: np.array([float])
26
           :type b: np.array([float])
           :type band: int
28
           :rtype: np.array([float])
30
           start_time = timeit.default_timer()
32
          # If the matrix, A, is banded, leverage that!
34
           if band is not None:
36
               self._band = band
          # If the matrix, A, is not square, exit
38
```

```
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```

```
if A. shape [0] != A. shape [1]:
               return "Matrix 'A' is not square!"
40
          n = A. shape [1]
42
44
          # Simultaneous Choleski factorization of A and chol-elimination
46
          # Choleski factorization & forward substitution
48
          for j in range(n):
50
              # If the matrix A is not positive definite, exit
52
              if A[j,j] \leq 0:
                   return "Matrix 'A' is not positive definite!"
54
              A[j,j] = A[j,j] ** 0.5
                                         # Compute the j, j entry of chol(A)
              b[j] /= A[j,j]
                                         # Compute the j entry of forward-sub
56
               for i in range (j+1, n-1):
58
                  # Banded matrix optimization
60
                   if (band is not None) and (i = self._band):
62
                       self._band += 1
                       break
64
                  A[i,j] /= A[j,j] # Compute the i, j entry of chol(A)
                  b[i] -= A[i,j] * b[j] # Look ahead modification of b
66
                   if A[i,j] == 0:
                                         # Optimization for matrix sparsity
68
                       continue
70
                   # Look ahead moidification of A
                   for k in range (j+1, i+1):
72
                      A[i,k] -= A[i,j] * A[k,j]
74
              # Perform computation for the test source
              if (j != n-1):
76
                  A[n-1,j] /= A[j,j]
                                          # Compute source entry of chol(A)
```

```
b[n-1] = A[n-1,j] * b[j] # Look ahead modification of b
78
                      # Look ahead moidification of A
                      for k in range (j+1, n):
80
                          A[n-1,k] -= A[n-1,j] * A[k,j]
82
84
            # Now solve the upper traingular system
86
            # Transpose(A) is the upper-tiangular matrix of chol(A)
88
            A[:] = matrix\_transpose(A)
90
            # Backward substitution
             for j in range (n - 1, -1, -1):
92
                b[j] /= A[j,j]
94
                 for i in range(j):
                     b[i] = \bar{A}[i,j] * b[j]
96
98
             elapsed_time = timeit.default_timer() - start_time
100
             if DEBUG:
                 print("Execution time:\n", elapsed_time, end="\n\n")
102
            # The solution was overwritten in the vector b
104
            return b
106
   if = name_{-} = "-main_{-}":
        from utils import generate_positive_semidef, matrix_dot_vector
108
110
        order = 10
        seed = 5
112
        print("\n", end="\n")
       print ( 'm' , end= '\n' )

print ("# — TEST — #", end="\n")

print ("# — Choleski Decomposition — #", end="\n")

print ("# — #", end="\n\n")
114
116
```

```
#", end="\n\n")

LISTING 5. choleski.py
```

chol_d = CholeskiDecomposition()

x = np.random.randn(order)
b = matrix_dot_vector(A=A, b=x)
print("A:\n", A, end="\n\n")

 $print("x:\n", x, end="\n\n")$

 $v = chol_d.solve(A=A, b=b)$

print("# -----

 $print("b (=Ax): \n", b, end="\n\n")$

118

120

122

124

126

128

Create a symmetric, real, positive definite matrix.

A = generate_positive_semidef(order=order, seed=seed)

 $print("2-norm\ error:\n",\ np.linalg.norm(v-x),\ end="\n'")$

 $print("result = solve(A, b):\n", v, end="\n\n")$

```
INNER_COORDINATES = (0.06, 0.08)
INNER_HALF_DIMENSIONS = (0.04, 0.02)
CONDUCTOR_POTENTIAL = 1.1e2
```

Listing 6. conductor_description.py