Solving Differential Equations on 2-D Geometries with Matlab

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I. INTRODUCTION

Here we introduce the reader to solving partial differential equations (PDEs) on 2 dimensional geometries using the Matlab package *PDE Tool.* This robust package solves PDE's using a finite element method. For more information on the finite element method, I refer you to Allyson or Dr. Gilmore ¹. If you want a cock-a-maymie explanation, you're welcome to come find me ².

II. SOLVING THE EIGENVALUES AND EIGENVECTORS ON A WASHER

A. Getting PDE Tool Ready to Go

Okay, so lets look at solving the actual problem given, which is solving the diffusion equation on a circular washer:

$$-\nabla \cdot (c * \nabla u) + a * u = \lambda * d * u$$

where c, a and d are constants and u is the solution. a is generally called k^2 and d is often called ρ , the weighting function. We wish to solve the Schrödinger equation specifically on the washer, so we have:

$$\frac{\hbar^2}{2m}\nabla^2\psi(r,\theta) = E\psi(r,\theta)$$

with the boundary conditions that $\psi = 0$ at the radial edges of the washer.

We will let our problem have "natural units," so $\hbar = m = 1$. So for us c = 0.5, a = d = 1.0. We'll need this later.

Start Matlab, then start the PDE tool by either finding in under the *Apps* tab or typing *pdetool* into the command window. You will be greeted with a blank screen under a row of buttons.

The screen is where we will draw our geometry, but first lets make it easier with a few settings. Click on *Options*, and turn on the Grid and Snap. Snap makes our drawings pop onto the grid lines you now see. Next select grid spacing and set it to draw grid lines at every integer in x and y. Also define the grid to go from $\begin{bmatrix} -12 & 12 \end{bmatrix}$ for both axes. Then click on *Axes Equal* to get the proper shape of the grid. Finally, click on *Solve*, then *Parameters* and set the Eigenvalue range to go from $\begin{bmatrix} 0 & 1 \end{bmatrix}$. If this range is too large it will time out while trying to solve for the eigenvalues.

B. Drawing the Geometry

Now that we have set the proper parameters, we can draw our geometry. Matlab uses a union/subtraction method to make complex geometries on the space. For instance, you can draw a disk, then draw a rectangle through it.

To draw a circle/ellipse, you pick either button that has an ellipse on it. The button with the '+' in the center means it draws starting the center at the point you click, while the other starts an edge of the shape where you click. The same goes for the rectangles.

You will see in the Set formula box that a combination of letters and numbers appears for each shape as you draw them, like for an ellipse E1 or for a rectangle R2. If these label your disk and rectangle, you can define your problem on both surfaces with E1 + R2 or just in the area of the disk outside of the rectangle with E1 - R2.

Here we want a washer. So first draw a circle with radius 12 by clicking on the button of an ellipse with the '+' in it, then clicking at the origin and dragging the circle out to a radius of 12. Then do this again for a circle of radius of 5. You should see in the *Set formula* box C1 + C2. Change this to C1 - C2, and you have defined the geometry of a washer.

C. Setting the Boundary Conditions and the Equation

Next we click on the $\partial\Omega$ button. This gives the boundary conditions, and you now see the washer shape outlined in red. If you double click any red line, it gives you the option to select Dirichlet or Neumann boundary conditions. The red is Dirichlet, Neumann would be blue. So this is already set to what we want, and no values need to be changed here.

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¹ Added to the list of people that know more than I do.

 $^{^2}$ Bring alcohol.



FIG. 1 The Matlab PDE Tool

Next click the *PDE* button, and the choices for the four different types of PDEs appear. Here Eigenvalue is the diffusion equation, which is what we want. You will see settings for the constants we defined before. Simply set c = 0.5, a = 0.0, and d = 1.0 and your done here.

D. Creating the Mesh and the Solution

Next click on the Δ button. This makes a mesh on the washer surface. This mesh is the FEM part of solving the problem. The initial mesh is fairly coarse, and will result in a rather coarse solution. Clicking the button with three Δ s stacked will refine the mesh for a more accurate solution, but takes longer to calculate. I recommend 3 times to make sure you get the proper degeneracy of the eignvalues.

After this, click on the *Mesh* in the menu bar, followed by *Jiggle Mesh*. This wiggles the mesh elements to better fit at the edges and bends in the geometry.

Finally, click the = button to solve the problem.

E. Solutions and Plots

After you click the solve button, Matlab will calculate the solution and then the window will change to a color plot of the first solution. You can then click the button that looks like a 3-D plot to explore the solutions. This will present you with the *Plot Selection* window. Here you can pick which eigenvector to plot by selecting the corresponding eigenvalue from the drop down menu on the bottom right, then checking which type of plot you want (color, contour, arrows, deformed mesh, or 3-D height plot). You can pick to plot the solution $u, \nabla u, |\nabla u|$, or some user defined function of u just as you would define any Matlab function.

If you simply click the different eigenvalues and then plot the color plots of u, you will be able to see all of the normal modes of the problem, including those that have degenerate eigenvalues.

You can then save the plots or click on *Solve* in the menu and then *Export Solution* to export the eigenvalues and eigenvectors to the main Matlab window for further plotting or work. You can also click on *File* then *Save as* to save an m-file of the problem and the solutions.

III. MY RESULTS

Having explained how to do the calculation, I now present my findings using *PDE Tool*. Note that I present the unitless eigenvalues λ , for the energies multiply these by \hbar^2/m . Here are the first 20 eigenvalues:

n	$\lambda * m/\hbar^2$
1	0.0989
2	0.1063
3	0.1063
4	0.1283
5	0.1283
6	0.1644
7	0.1644
8	0.2136
9	0.2136
10	0.2748
11	0.2748
12	0.3470
13	0.3470
14	0.4012
15	0.4092
16	0.4092
17	0.4291
18	0.4291
19	0.4334
20	0.4334

The degeneracy in the eigenvalues relates to the axial symmetry of the washer shape. It doesn't matter if I travel the washer in the positive or negative θ direction, I

still see the same infinite potentials at the same radii. So I get an energy for travel clockwise $exp(+in\theta)$ and counterclockwise $exp(-in\theta)$. There are two singular eigenvalues here though, the ground state (n=1) and the fourteenth state (n=14). These are states that don't have nodes in the *theta* direction, instead they have nodes in the radial r direction. We anticipate these would continue to appear as n gets higher, with each singular eigenvalue corresponding to an eigenfunction with an additional radial node.

The plots of the degenerate wave functions show that they are just rotations about the central axis of the washer, representing the fact that they come from the symmetry in this coordinate. The nodes are highlighted by the contour lines which are plotted on the graphs and show where the "barriers" are in the wave function.

IV. CONCLUSION

So there you have it, we have solved the problem. This general method is the method for solving all 2-D PDEs with the PDE tool in Matlab. Hopefully this has been of some help in how to do this!

Happy Matlabbing!

REFERENCES

Wikipedia, (2014), "Finite element method — Wikipedia, the free encyclopedia," [Online; accessed 22-April-2014].



FIG. 2 The wave function for n=1 (ground state).



FIG. 3 The wave function for n=2.



FIG. 4 The wave function for n=3.



FIG. 5 The wave function for n=4.



FIG. 6 The wave function for n=5.



FIG. 7 The wave function for n=5.



FIG. 8 The wave function for n=6.



FIG. 9 The wave function for n=7.



FIG. 10 The wave function for n=14. Note the radial node that appears.