ORNL Summer Project Report

Simulation of Composites Structure in Bone

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1. Introduction

The PDE to be solved is

$$\text{(BVP1)} \begin{cases} \nabla \cdot [(\epsilon_1 \chi_1(\boldsymbol{x}) + \epsilon_2 \chi_2(\boldsymbol{x}))\nabla\phi] &= 0, \\ \phi|_{\partial\Omega} &= \sum_{j=1}^{d} E_j^0 x_j \end{cases} \tag{1}$$

In this project, we aim at solving the above PDE where χ_1 is the characteristic function for trabecula and χ_2 is the characteristic function for marrow.

After solving the PDE, the results will be used to evaluate the effective dielectric properties which is defined by

$$\epsilon_{ik}^* \stackrel{\text{def}}{=} \int_{\Omega} [\epsilon_1 \chi_1(\boldsymbol{x}) + \epsilon_2 \chi_2(\boldsymbol{x})] \partial_i \phi \, d\boldsymbol{x}$$

with $E_j^0 = \delta_{kj}$

Let $\epsilon_1(\omega) = 1 \quad \frac{\omega_p^2}{\omega(\omega + i\gamma)}$, where $\omega_p = 9.4 \times 10^5 \, s^{-1}$, $\gamma = 4 \times 10^5 \, s^{-1}$. We chose $\epsilon_2 = 1.96$. Our goal is to evaluate the effective dielectric properties with different values of ω between 10^5 and 10^6.

A code BIBLAP is written to solve this specific problem. In this code, Boundary Element Method is used to solve the PDE. Part of this code is modified from SCBLAP-1.0.

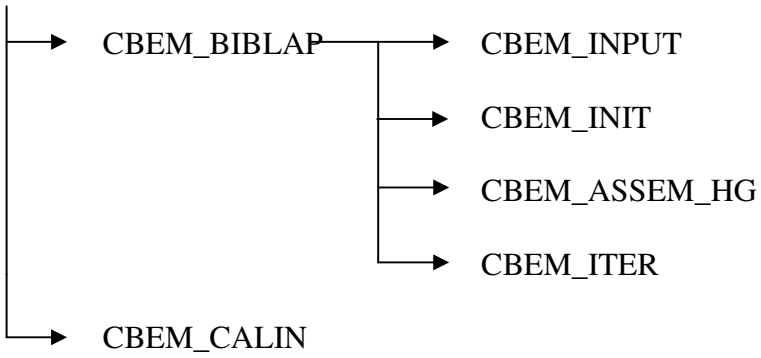
2. Structure of BIBLAP

BIBLAP contains various routines to deal with different jobs when solving the PDE. Here's the description of each routines:

Routine	Description
CBEM_INPUT	Read input data and parameters
CBEM_INIT	Initialize parameters
CBEM_ASSEM_HG	Assemble h and g influence matrices
CBEM_ITER	Iterate for the interface potentials and fluxes
CBEM_CALIN	Calculate the value inside the boundary

CBEM_INIT is directly used from SCBLAP-1.0 while others are modified or new from SCBLAP.

MAIN PROGRAM



3. Solution of Box-in-box Laplace Equation by BIBLAP

i. **Iteration**

To solve the PDE

$$(\text{BVP1}) \begin{cases} \nabla \cdot [(\epsilon_1 \chi_1(\boldsymbol{x}) + \epsilon_2 \chi_2(\boldsymbol{x}))\nabla\phi] &= 0, \\ \phi|_{\partial\Omega} &= \sum_{j=1}^{d} E_j^0 x_j \end{cases}$$

The domain is separated into 2 parts Ω_1, Ω_2 which represents “Trabecula” and ”Bone Marrows” respectively. In this case, the original PDE becomes two seperate Laplace eqautions on different domains. So, if the boundary values of each region are known, SCBLAP-1.0 can be used to solve the PDE.

In addition, transmission conditions hold on the interface in the problem.

$$(\text{TC}) \begin{cases} \phi_1 = \phi_2 \\ -\epsilon_1 \frac{\partial \phi_1}{\partial \hat{n}_1} = \epsilon_2 \frac{\partial \phi_2}{\partial \hat{n}_2} \end{cases}$$

Boundary condition of Ω_2 is prescribed but boundary condition of Ω_1 is unknown. Thus, iteration is used to find the values at the interface.

$$\Omega = \Omega_1 \cup \mathcal{I} \cup \Omega_2$$

with interface $\mathcal{I} := \overline{\Omega_1} \cap \overline{\Omega_2}$

Step 1 : Prepare the input file such that the meshes for inner region (Ω_1) appear first.

Step 2 : Make initial guess for values of flux, i.e. $\dfrac{\partial \phi_2}{\partial n_2}$ on $\mathcal{I}$.

$$\left.\frac{\partial \phi_2}{\partial n_2}\right|_{\mathcal{I}} = g_0 = 0$$

Step 3 : Solve the mix-outer-problem

$$\text{(BVP-outer)} \begin{cases} \triangle \phi_2 = 0 \text{ in } \Omega_2 \\ \phi_2|_{\partial\Omega} = \sum_{j-1}^{d} E_j^0 x_j, \\ \frac{\partial \phi_2}{\partial n_2}|_{\mathcal{I}} - g_0 \end{cases} \tag{3}$$

Step 4 : Use the transmission condition on $\mathcal{I}$: $\phi_1 = \phi_2$ to find the boundary condition for the inner problem.

Step 5 : Solve the inner-problem

$$\text{(BVP-inner)} \begin{cases} \triangle \phi_1 = 0 \text{ in } \Omega_1 \\ \phi_1 = \phi_2 \text{ on } \partial\Omega_1 \end{cases} \tag{4}$$

Step 6 : Use the other transmission condition

$$\epsilon_1 \frac{\partial \phi_1}{\partial n_1} - -\epsilon_2 \frac{\partial \phi_2}{\partial n_2}$$

to calculate the boundary value of ϕ_2 on $\mathcal{I}$. Here n_i is outer normal for region Ω_i, $i = 1, 2$.

Step 7 : Go to Step 1.

After finding the interface value, part of SCBLAP (FIELDEVAL) can be used to evaluate the values inside.

ii. **Matrix H and G**

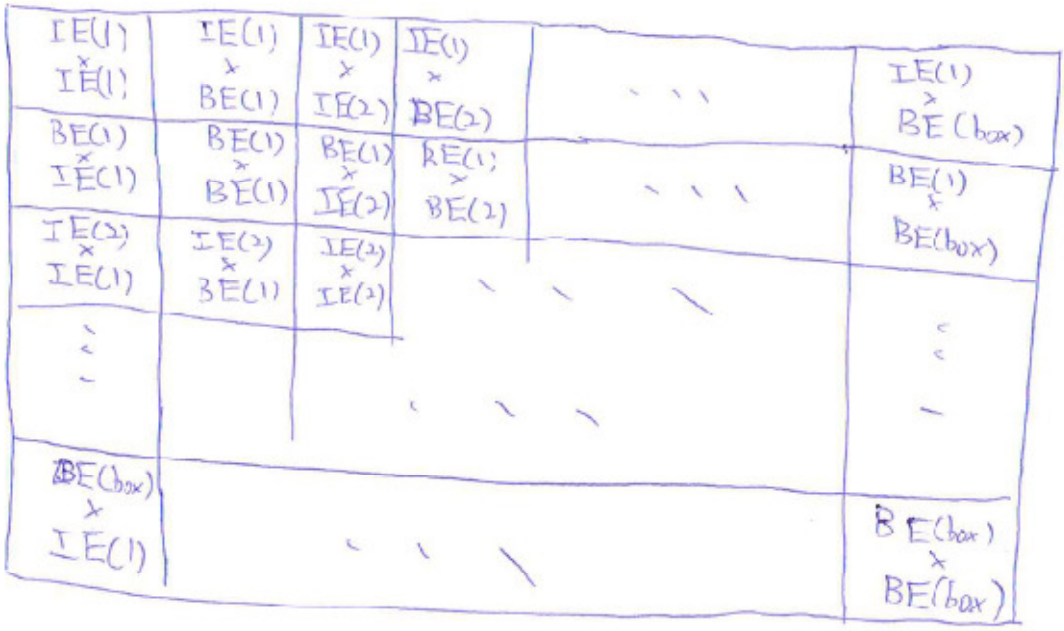
To do the iteration, matrix H and G which are defined as below are required.

$$G_{ij} = \lim_{x_\varepsilon \to x^i} g_j(x_\varepsilon), \quad H_{ij} = \lim_{x_\varepsilon \to x^i} h_j(x_\varepsilon), \quad x^i \in \Gamma_i$$

with the single-layer potential g_j and double-layer potential h_j expressed as

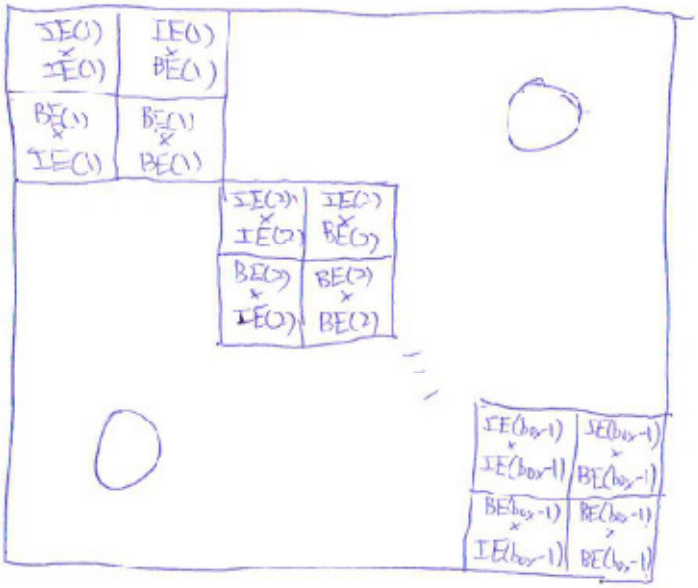
$$g_j(\boldsymbol{x}) = \int_{\Gamma_j} G(\boldsymbol{x}, \boldsymbol{y})\, d\Gamma_y, \quad h_j(\boldsymbol{x}) = \int_{\Gamma_j} \boldsymbol{H}(\boldsymbol{x}, \boldsymbol{y}) \cdot \boldsymbol{n}(\boldsymbol{y})\, d\Gamma_y, \quad \boldsymbol{x} \in \mathbb{R}^3.$$

Firstly, H and G for all the elements are calculated. Then, H and G have format as below:

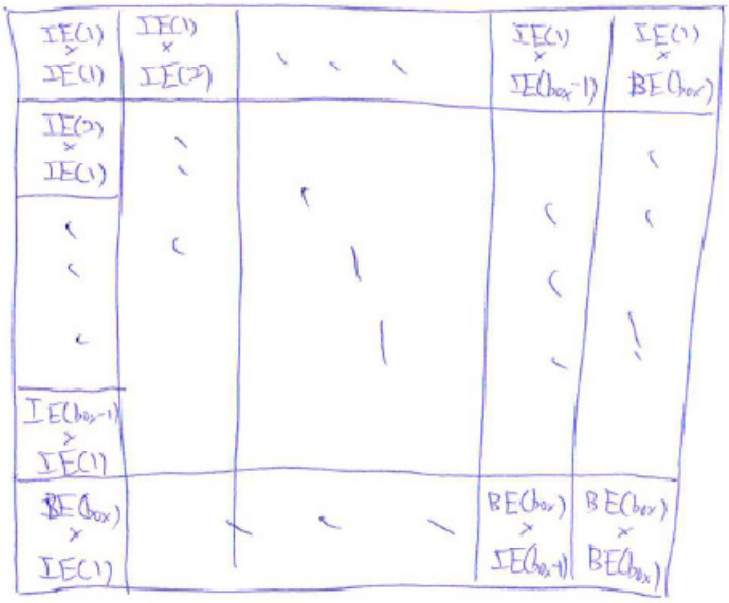


where IE(k) means Γ_i is extracted from the interface elements of the k-th box and BE(k) means Γ_i is extracted from the boundary elements of the k-th box

Then, Hi, Gi,(for inner region) Hn and Gn (for outer region) are extracted from G and H. Format of Hi, Gi



Format of Hn, Gn



iii. **Energy Norm and Effective Dielectric Property**

Energy norm can be calculated by using only boundary and interface potentials.

$$E = \int_{\Omega} \nabla\cdot\left(\phi\cdot(\varepsilon_1\chi_1(x)\nabla\phi(x)+\varepsilon_2\chi_2(x)\nabla\phi(x))\right)dx$$

$$= \int_{\Omega_1} \varepsilon_1\cdot\nabla\cdot(\phi\nabla\phi)\,dx + \int_{\Omega_2}\varepsilon_2\cdot\nabla\cdot(\phi\nabla\phi)\,dx$$

$$= \int_{\partial\Omega_1}\varepsilon_1\phi\,(\nabla\phi\cdot\hat{n}_1)\,dS + \int_{\partial\Omega_2}\varepsilon_2\cdot\phi\,(\nabla\phi\cdot\hat{n}_2)\,dS$$

$$= \int_{\partial\Omega_1}\varepsilon_1\phi\cdot\frac{\partial\phi}{\partial\hat{n}_1}\,dS + \int_{\partial\Omega_2}\varepsilon_2\cdot\phi\cdot\frac{\partial\phi}{\partial\hat{n}_2}\,dS$$

Similarly, effective dielectric property can also be evaluated by using boundary and interface values.

$$\varepsilon^*_{ik} = \int_{\Omega}(\varepsilon_1\chi_1(x)+\varepsilon_2\chi_2(x))\partial_i\phi\,dx$$

$$= \int_{\Omega}(\varepsilon_1\chi_1(x)+\varepsilon_2\chi_2(x))(\vec{e}_i\cdot\nabla\phi)\,dx$$

$$= \int_{\Omega}(\varepsilon_1\chi_1(x)+\varepsilon_2\chi_2(x))\nabla\cdot(\phi\vec{e}_i)\,dx$$

$$= \int_{\partial\Omega_1}\varepsilon_1\phi\,\vec{e}_i\cdot\hat{n}_1\,dS + \int_{\partial\Omega_2}\varepsilon_2\phi\,\vec{e}_i\cdot\hat{n}_2\,dS$$

4. How to Use BIBLAP

To use BIBLAP, two input files are required. Firstly, the dielectric coefficient, surface mesh and boundary condition data should be provided in the file “bndata.dat”. Secondly, the points which are interested to evaluate the values should be provided in “indata.dat”.

i. <u>Format of input files:</u>

“bndata.dat”

Number of Boxes (box)
Epsilon_1
Epsilon_2
Number of Nodes
Number of Interface Elements on the first box
Number of Interface Elements on the second box
. . .
Number of Boundary Elements on the first box
Number of Boundary Elements on the second box
. . .
Number of Boundary Elements on the Outermost Box
. . . Vertices (x y z) . . .
. . . Element Connectivity and Boundary Condition(for boundary elements) (i j k xxxxx m) . . .

"indata.dat"

Number of Vertices inside the First Box
Number of Vertices inside the Second Box
. . .
Number of Vertices inside the Outermost Box
. . . Vertices (x y z) . . .

In "bndata.dat", for the outermost box, only the number of boundary elements are required. Moreover, "Vertices" means the x-, y-, z-coordinates of each vertex.

"Element Connectivity" represents the vertices which form the triangle, for example, "1 3 4" means the first, third and forth vertices listing in the "Vertices" part form a triangle. The connectivity should be arrange such that the normal of each boundary element (which is defined by right-hand grid rule) points outward where that of each interface element points inward. In addition, the element connectivity should be arranged in the order "Interface element of first box", "Boundary element of first box", "Interface element of second box", "Boundary element of second box", … , "Boundary element of outermost box".

For those triangles lying on the boundary, "Boundary Condition" is required. "Boundary Condition" is represented by 2 numbers. The first number (xxxxx) is the value of either Dirichlet data or Neumann data. The second one (m) can either be 0 or 1 where 0 means the prescribed data is Dirichlet data and 1 means Neumann data.

In "indata.dat", "Vertices" should be arranged in the order of "Vertices inside the first box", "Vertices inside the second box", …, " Vertices inside the outermost box".

ii. <u>Preparation of Input File</u>

To make the file bndata, various steps have to be done to obtain the meshing from the micro-CT scan of the bone image.

Step 1

Transform the image to Black and White image which has logical values 0 and 1 respectively

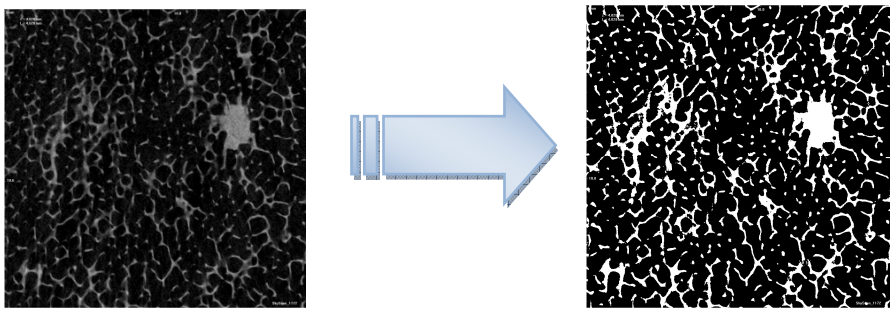


Figure (i) Raw to Black and White

Step 2

Stack up the images by the MATLAB code ‘stack.m’ (2).
Number of images and X/Y-cut are required for input. The output of the function is a 3-d array storing the smooth volume data. Sample input: data=stack (100,200), then data is the output volume data, 100 is the number of images used and 200 is X,Y-cut.

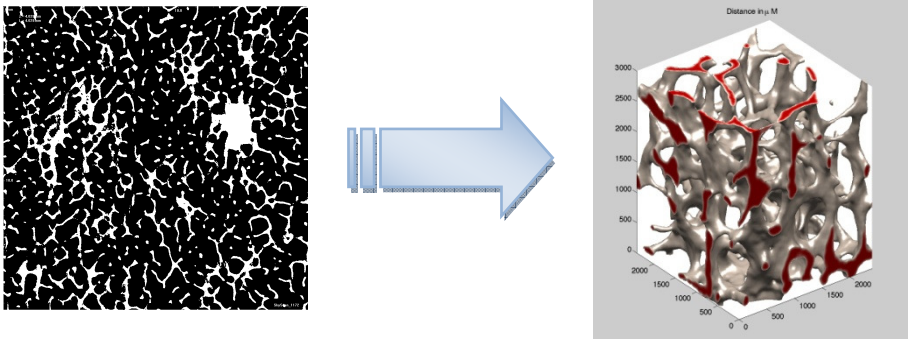


Figure (ii) Stack up

Step 3

Get the facet file of the trabecula by the MATLAB code ‘facet.m’ (3).
The volume data is required for input, e.g., facet(data). Two output file named ‘trab_bn.fac’ and ‘trab_in.fac’ representing the boundary and interface elements respectively are generated.

Step 4

Import the two surfaces to CUBIT. Remember to stitch the surface.

Step 5

Mesh the two surfaces simultaneously.
Select Meshing→Surface→Interval. The larger the Interval size, the finer the mesh generated. Then select Mesh→Trimesh→Apply Scheme→Apply

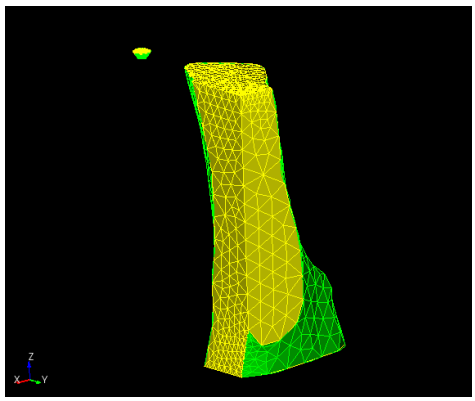


Figure (iii) Meshed Trabecula

Step 6

Convert the mesh to ACIS file

Add all surface mesh into a block and export it as ‘Genesis’ file. Then, open a new file and import the Genesis file. This time, export the mesh in STL file. Lastly, convert the STL file to ACIS file by the MATLAB code ‘Convert_stl_to_sat.m’ (4). The STL filename is required for input, e.g., Convert_stl_to_sat(“sample.stl”)

Step 7

Import the ACIS file and create a brick with size catering to the trabecula.

Step 8

Imprint the trabecula to the brick

Select Geometry→Volume→Imprint Merge→Tolerant Imprint. Set a proper tolerance and fill in the volume id of both trabecula and the brick.

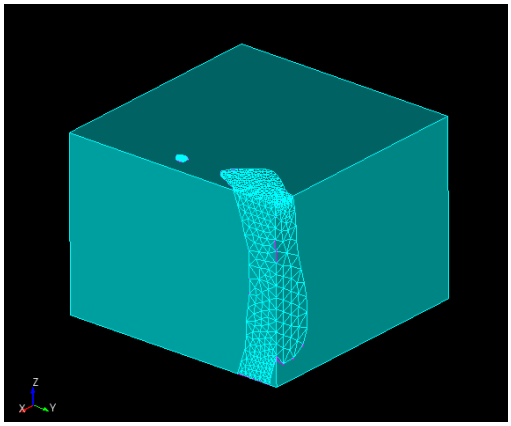


Figure (iv) Imprinted Brick

Step 9

Mesh the brick

Select Meshing→Surface→Interval→Auto.

Then, select Mesh→Trimesh→Apply Scheme→Apply

At last, Exclude the intersection of the brick and the trabecular.

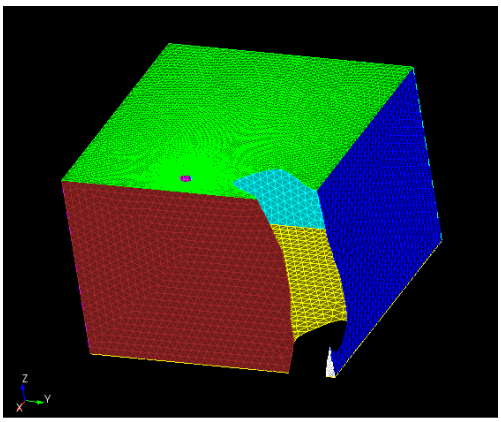


Figure (v) Meshed Brick

Step 10

Export the mesh to facet file and use excel or MATLAB to arrange the order.

For indata, an arbitrary grid can be used. However, the number of vertices inside the k-th box must be specified and the grid points should be in the order mentioned above. One possible method to test the position of the grid point is setting constant boundary (say 1) and assuming all the grid points to be in the same region. Then, run the code. In the file output'invalue.dat', if the value is very close to 1, the grid point falls in the region assumed. If the value is very close to 0, the grid point falls in the region assumed. If the value is neither close to 0 nor 1 or the value is 1 at all the region, the grid point is very close to the boundary. In this case, it is better to remove that point.

iii. Getting started with BIBLAP

On a Linux system with fortran90 compiler, BLAS and LAPACK installed. The prospective users should (i) unzip the file BIBLAP-x.tar (x is the version number), edit the file 'makefile', (iii) issue make. The first step can be accomplished by typing "tar -zxvf scblap.tgz" in the shell. In the second part, open the 'makefile' with a text editor and replace gfortran by the Fortran 90 compiler on your system. The third step simply generates an executable called 'lapEx'.

Then, move the two input file, 'bndata.dat' and 'indata.dat' into the same file of 'lapEx'. Lastly, simply run the executable 'lapEx'.

5. Results

There are altogether three cases tested. In each case, constant boundary (phi = 1) is used to test at first. The results in all cases are very nice, where all the potentials and fluxes are very close to 1 and 0 respectively. After testing with constant boundary, some specific cases which can be analyzed quite easily have been done. The followings are the results of specific test cases.

1. **Sphere-in-sphere with Boundary Condition phi=z/r, e_1=0.4, e_2=1.96**

   In this case, the exact form of the solution can be found. The CBEM solution is quite accurate. (Refer to attachment (1)) Following are some graphs of the results:

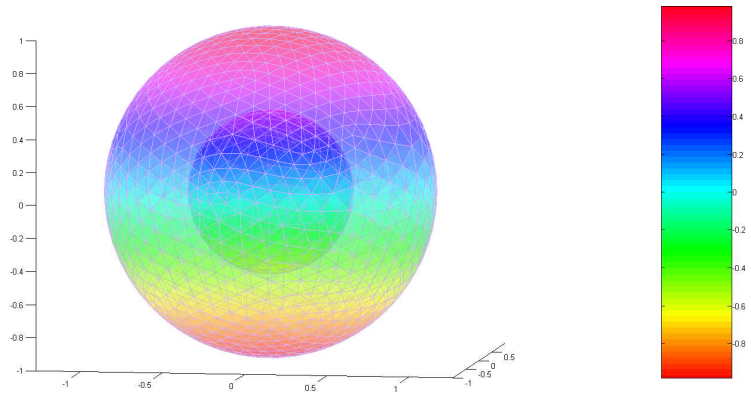


Figure (vi) Sphere-in-sphere

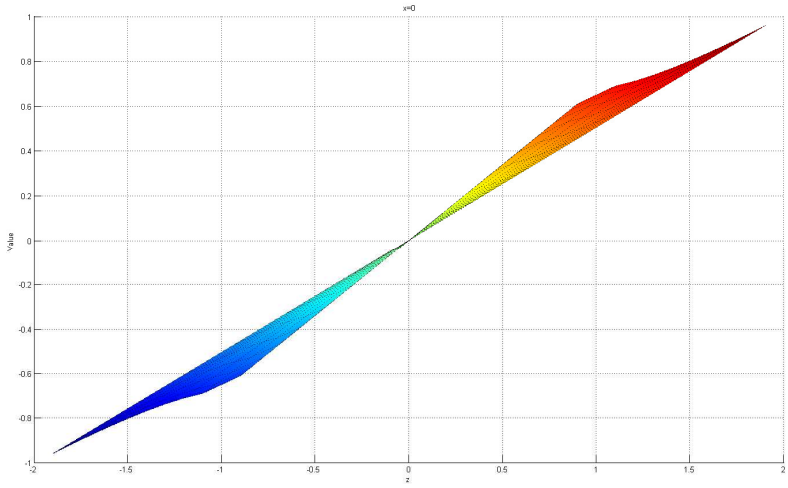


Figure (vii) Cross-sectional view at x=0

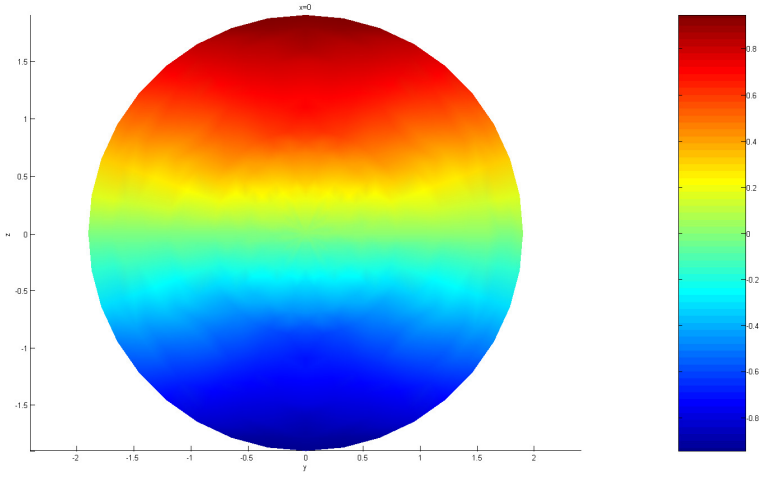


Figure (viii) Cross-sectional view at x=0 (ii)

In Figure (vii), it's quite obvious that the normal derivative is discontinuous at the interface. This is because of the conservation of flux with different epsilon.

In Figure (viii), the potential of the points are proportional to z consistent to the exact solution phi=k_1z in the outer region and phi=k_2z in the inner region for some constant k_1, k_2.

2. **<u>A 5x5x10 Rectangular Pole in a 10x10x10 Cube with e_1=0.3, e_2=1.96</u>**

In this case, we use the rectangular pole to simulate the trabecula. Three different boundary conditions (a) phi = x, (b) phi = y, (c) phi =z have been tried. The energy in each case and the effective dielectric property have been evaluated.

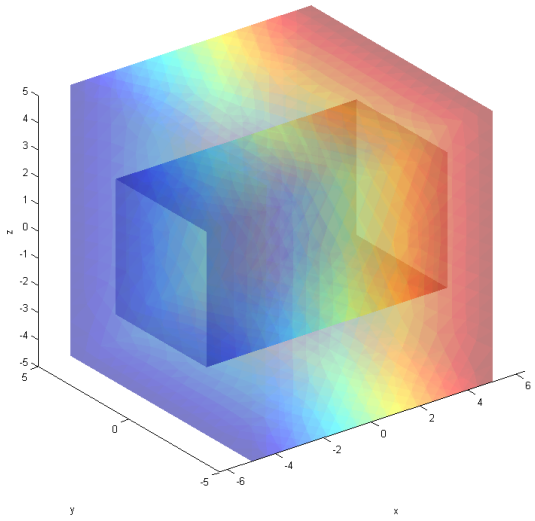


Figure (iv) Cube with a Pole

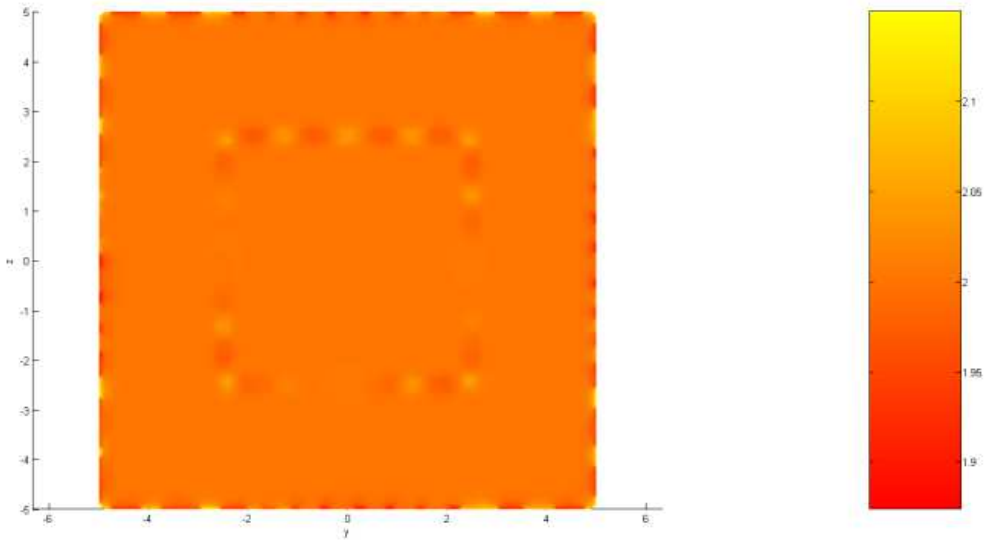


Figure (v) Cross-sectional View at x=2 with BC phi=x

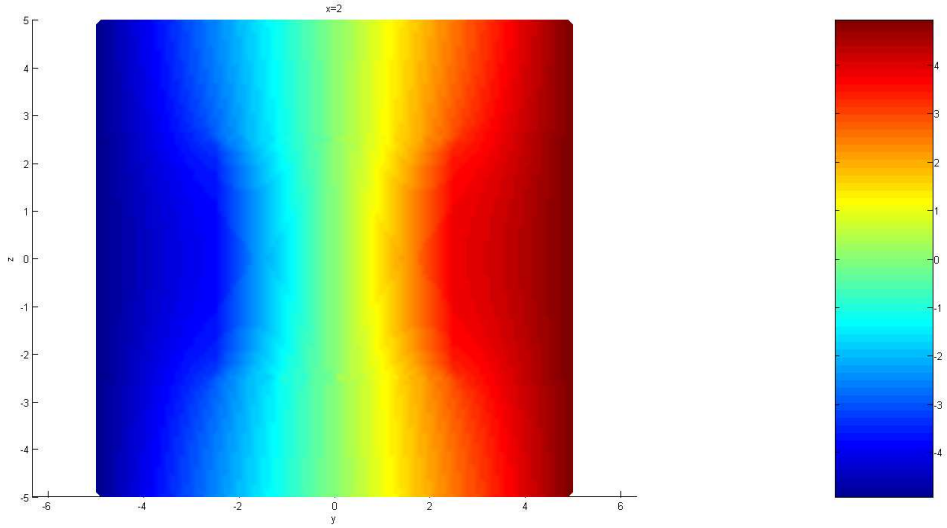


Figure (vi) Cross-sectional View at x=2 with BC phi=y

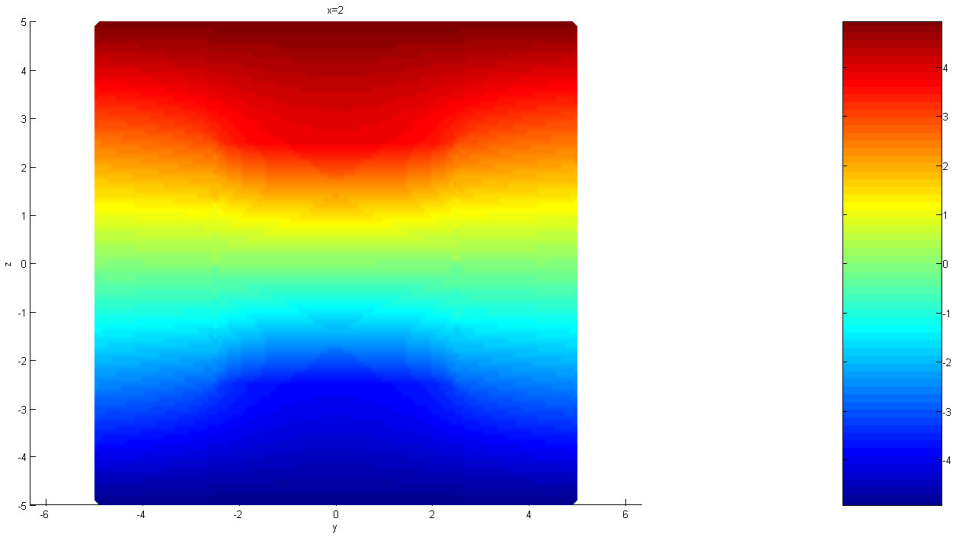


Figure (vii) Cross-sectional View at x=2 with BC phi=z

In Figure (v), the value at the cross-sectional area should be exactly 2 as the exact solution for this Boundary Condition is phi = x everywhere. However, the points which are very close to the boundary leading to some error so the graph seems not very smooth.

For Figure (vi) and (vii), the results is as expected. The potential 'collapses' to the centre along the y- and z- direction respectively.

In this test case, the effective dielectric property is

$$\mathbf{e}^{*} = \begin{pmatrix} 1545.00000000 & -0.00070677 & 0.00007320 \\ 0.02045203 & 1378.82395050 & 0.00954151 \\ 0.01787377 & 0.00936246 & 1378.81195063 \end{pmatrix}$$

3. Real Trabecula and Marrow

A small piece of trabecula is used in this test case. The following are the results

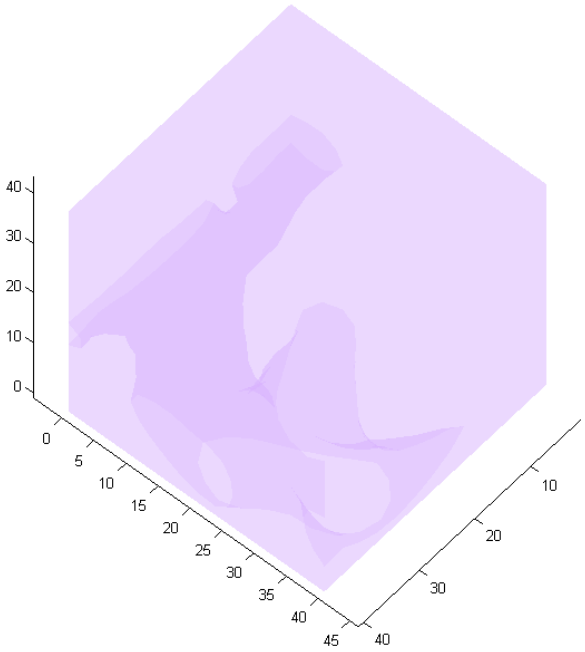


Figure (viii) Trabecula and Marrow

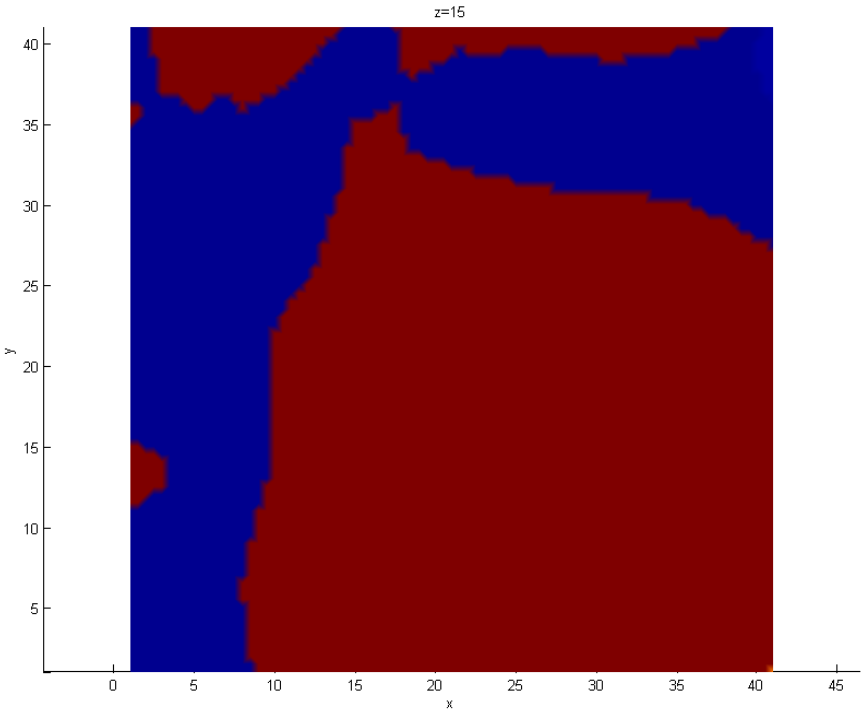


Figure (ix) Cross-sectional View at z = 15 (Blue = Trabecula, Red = Marrow)

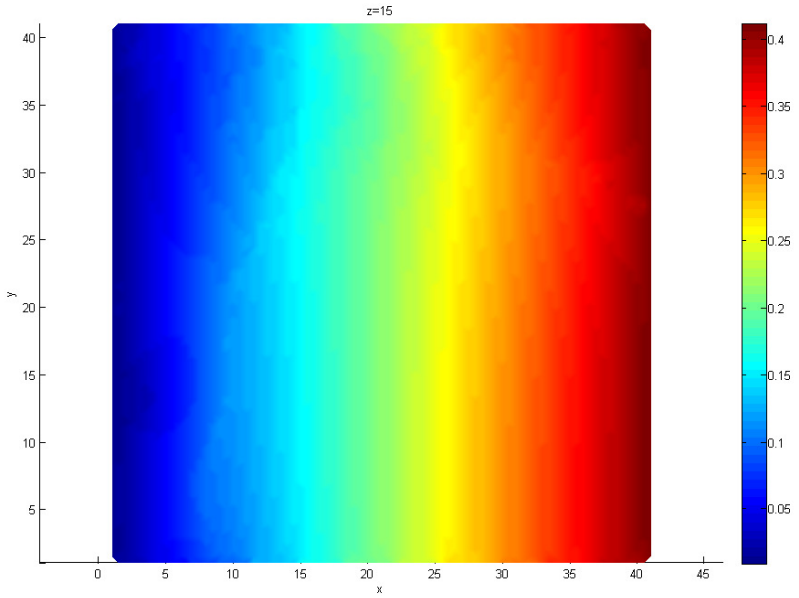


Figure (xv) Cross-sectional View at z = 15 with BC phi = x/100

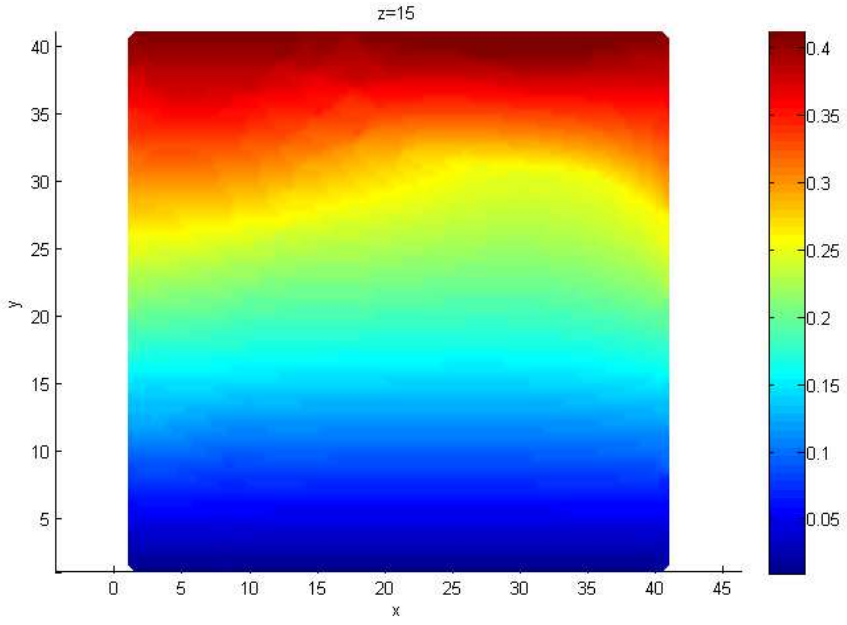


Figure (xvi) Cross-sectional View at z = 15 with BC phi = y/100

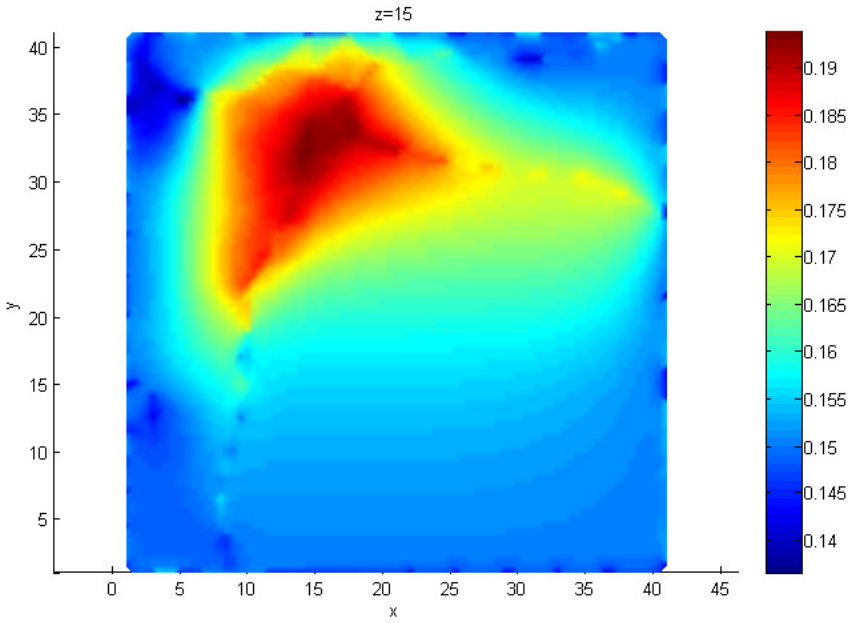


Figure (xvii) Cross-sectional View at z = 15 with BC phi = z/100

In this case, the effective dielectric properties is

$$\mathbf{e}^{*} = \begin{pmatrix} 1073.13390244 & -11.77431308 & -6.95933796 \\ -2.58523184 & 1052.90200676 & 14.87521832 \\ -2.96664855 & 13.85313748 & 1058.79303154 \end{pmatrix}$$

6. Future Work

1. Visualization
   As shown in the above results, the boundary and interface of the cross-sectional area is not smooth enough since the equation used to evaluate the values of inner point doesn't hold for points on the boundary.
   One possible improvement is to use CUBIT to generate the grid points such that none of the points fall on (or very close to) the boundary or interface.

2. Large Scale Trabecula
   A much larger scale of trabecula model should be used for the simulation as it will be more similar to the real case. However, to do a large model, large memory is needed to store the matrices H and G. For my computer(4Gb RAM), it can only deal with ~8000 triangles.

3.

Part II: Computing the spectrum of the microstructure

The problem to be solved is: Find $(\lambda, \mathbf{v} \subset (L^2(\Omega))^d)$ such that

$$\nabla \triangle^{-1} \nabla \cdot (\chi_2 \mathbf{v}) - \lambda \mathbf{v}$$

Part III: Computing Permeability of cancellous bone sample

It will be based on the Navier-Stokes equations in the fluid (bone marrow) domain

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\, \mathbf{u} - \nu \triangle \mathbf{u} = \frac{1}{\rho} \nabla p$$

Attachment:

(1) Results.tgz (Test Results)
(2) stack.m
(3) facet.m
(4) STL_to_SAT_conversion.zip (Convert_stl_to_sat.m)
(5) BIBLAP-1.2.tgz