CSE 397 Introduction to Computational Oncology
Homework 2 - Modeling Avascular Growth

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1) Derive the FDM description for an interior node for the mechanical equilibrium in terms of displacement in the x-direction (U_x) and y-direction (U_y). Use the relations for stress and the definitions for strain.

Beginning with the definition of strain and the centered difference method,

$$\begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ 2\varepsilon_{xy} \end{bmatrix} = \begin{bmatrix} \dfrac{\partial U_x}{\partial x} \\ \dfrac{\partial U_y}{\partial y} \\ \dfrac{\partial U_x}{\partial y} + \dfrac{\partial U_y}{\partial x} \end{bmatrix}$$

$$= \begin{bmatrix} \dfrac{U_x(x+\Delta x, y) - U_x(x-\Delta x, y)}{2\Delta x} \\ \dfrac{U_y(x, y+\Delta y) - U_y(x, y-\Delta y)}{2\Delta y} \\ \dfrac{U_y(x+\Delta x, y) - U_y(x-\Delta x, y)}{2\Delta x} + \dfrac{U_x(x, y+\Delta y) - U_x(x, y-\Delta y)}{2\Delta y} \end{bmatrix}$$

Next, the stress components:

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \end{bmatrix} = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & (1-2\nu)/2 \end{bmatrix} \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ 2\varepsilon_{xy} \end{bmatrix}$$

$$\sigma_{xx} = \frac{E}{(1+\nu)(1-2\nu)} \left[(1-\nu) \left(\frac{U_x(x+\Delta x, y) - U_x(x-\Delta x, y)}{2\Delta x} \right) + \nu \left(\frac{U_y(x, y+\Delta y) - U_y(x, y-\Delta y)}{2\Delta y} \right) \right]$$

$$\sigma_{yy} = \frac{E}{(1+\nu)(1-2\nu)} \left[\nu \left(\frac{U_x(x+\Delta x, y) - U_x(x-\Delta x, y)}{2\Delta x} \right) + (1-\nu) \left(\frac{U_y(x, y+\Delta y) - U_y(x, y-\Delta y)}{2\Delta y} \right) \right]$$

$$\sigma_{xy} = \frac{E}{2(1+\nu)} \left[\frac{U_y(x+\Delta x, y) - U_y(x-\Delta x, y)}{2\Delta x} + \frac{U_x(x, y+\Delta y) - U_x(x, y-\Delta y)}{2\Delta y} \right]$$

Finally, we can use the stress-strain relationships to determine the strains based on the gradient of the number of cells:

$$\nabla \cdot \begin{bmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{yx} & \sigma_{yy} \end{bmatrix} = \lambda_1 \nabla N$$

$$\begin{bmatrix} \dfrac{\partial \sigma_{xx}}{\partial x} + \dfrac{\partial \sigma_{xy}}{\partial y} \\ \dfrac{\partial \sigma_{yx}}{\partial x} + \dfrac{\partial \sigma_{yy}}{\partial y} \end{bmatrix} = \lambda_1 \begin{bmatrix} \dfrac{\partial N}{\partial x} \\ \dfrac{\partial N}{\partial y} \end{bmatrix}$$

Where the first derivatives of the stress components are second derivatives of the strain components using the previous relationship:

$$
\begin{aligned}
\frac{\partial \sigma_{xx}}{\partial x} &= \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)\left(\frac{\partial^2 U_x}{\partial x^2}\right) + \nu\left(\frac{\partial^2 U_y}{\partial x \partial y}\right)\right] \\
&= \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)\frac{U_x(x+\Delta x, y) - 2U_x(x,y) + U_x(x-\Delta x, y)}{\Delta x^2}\right. \\
&\qquad \left. + \nu \frac{U_y(x+\Delta x, y+\Delta y) - U_y(x+\Delta x, y-\Delta y) - U_y(x-\Delta x, y+\Delta y) + U_y(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}\right] \\
\frac{\partial \sigma_{xy}}{\partial y} &= \frac{E}{2(1+\nu)}\left[\frac{\partial^2 U_y}{\partial x \partial y} + \frac{\partial^2 U_x}{\partial y^2}\right] \\
&= \frac{E}{2(1+\nu)}\left[\frac{U_y(x+\Delta x, y+\Delta y) - U_y(x+\Delta x, y-\Delta y) - U_y(x-\Delta x, y+\Delta y) + U_y(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}\right. \\
&\qquad \left. + \frac{U_x(x, y+\Delta y) - 2U_x(x,y) + U_x(x, y-\Delta y)}{\Delta y^2}\right] \\
\frac{\partial \sigma_{yx}}{\partial x} &= \frac{E}{2(1+\nu)}\left[\frac{\partial^2 U_y}{\partial x^2} + \frac{\partial^2 U_x}{\partial x \partial y}\right] \\
&= \frac{E}{2(1+\nu)}\left[\frac{U_y(x+\Delta x, y) - 2U_y(x,y) + U_y(x-\Delta x, y)}{\Delta x^2}\right. \\
&\qquad \left. + \frac{U_x(x+\Delta x, y+\Delta y) - U_x(x+\Delta x, y-\Delta y) - U_x(x-\Delta x, y+\Delta y) + U_x(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}\right] \\
\frac{\partial \sigma_{yy}}{\partial y} &= \frac{E}{(1+\nu)(1-2\nu)}\left[\nu\left(\frac{\partial^2 U_x}{\partial x \partial y}\right) + (1-\nu)\left(\frac{\partial^2 U_y}{\partial y^2}\right)\right] \\
&= \frac{E}{(1+\nu)(1-2\nu)}\left[(1-\nu)\frac{U_x(x+\Delta x, y) - 2U_x(x,y) + U_x(x-\Delta x, y)}{\Delta x^2}\right. \\
&\qquad \left. + \nu \frac{U_x(x+\Delta x, y+\Delta y) - U_x(x+\Delta x, y-\Delta y) - U_x(x-\Delta x, y+\Delta y) + U_x(x-\Delta x, y-\Delta y)}{4\Delta x \Delta y}\right]
\end{aligned}
$$

And the gradient of the cell population is:

$$
\begin{bmatrix} \dfrac{\partial N}{\partial x} \\ \dfrac{\partial N}{\partial y} \end{bmatrix} = \begin{bmatrix} \dfrac{N(x+\Delta x, y) - N(x-\Delta x, y)}{2\Delta x} \\ \dfrac{N(x, y+\Delta y) - N(x, y-\Delta y)}{2\Delta y} \end{bmatrix}
$$

2) Four Matlab functions:

2a) To reshape the displacement vector into a 3D matrix, the matlab function **reshape** was used.

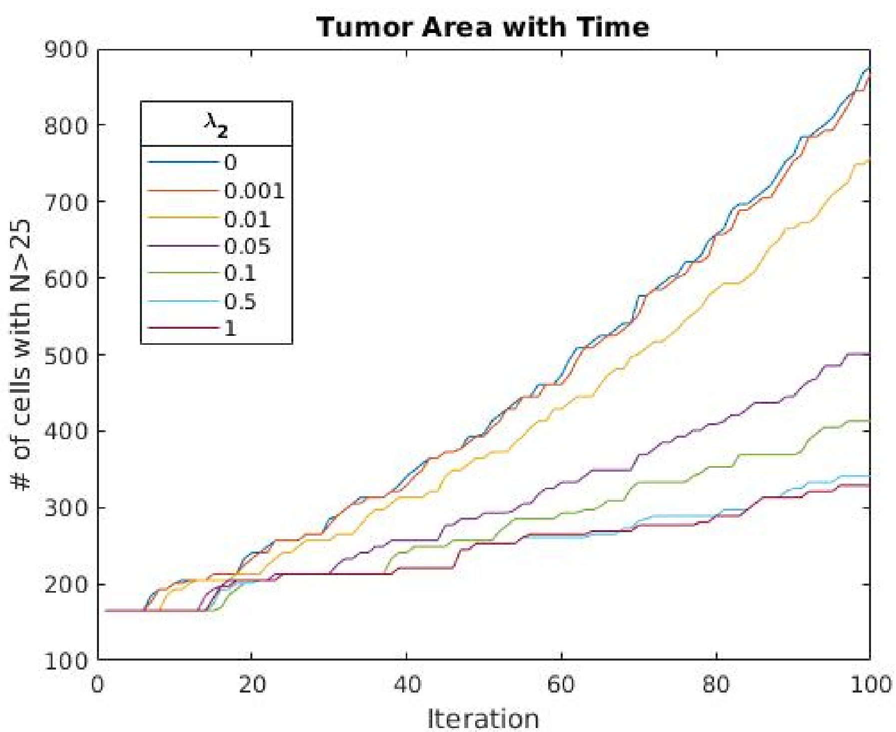
2b) The gradient was calculated using center differences above for interior nodes and 0 for boundary nodes. The resulting matrix was reshaped into a vector.

2c) The strains were calculated using the center differences above for interior nodes and forward/backward differences for boundary nodes.

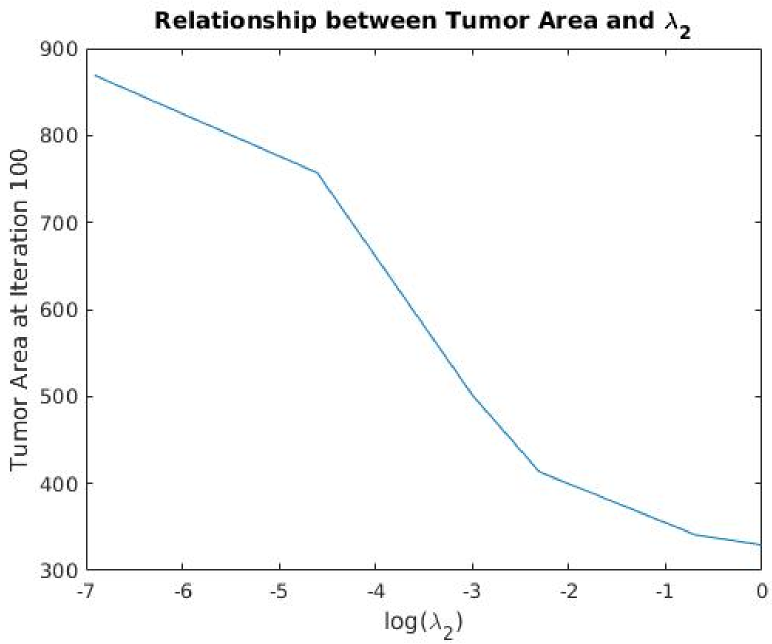
2d) The stresses were calculated using the constitutive equations above, and then the Von Mises stresses at each node were calculated.

3) Simulations:

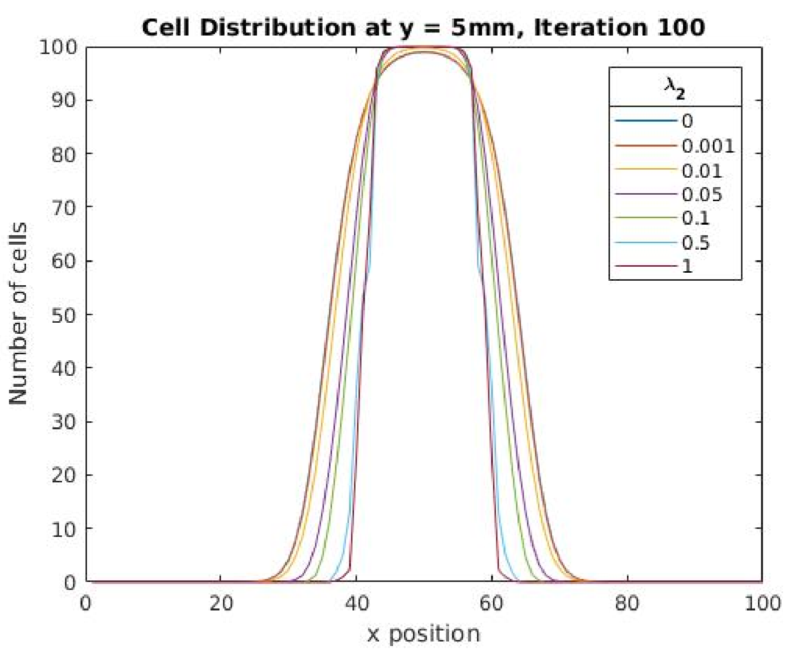
3a)



It can be seen in the first two plots that an increase in the λ_2 parameter decreases the tumor area. This is to be expected since an increase in the fitting term λ_2 causes a decrease in the diffusion coefficient since the Von Mises stress is strictly positive. For example, if $\lambda_2 = 0$, $D = D_0$, while if $\lambda_2 = 1$, $D = D_0 e^{-\sigma_{vm}}$.



3b)



A larger λ_2 parameter means the stresses have a greater effect on the diffusion of tumor cells, restricting their movement. Thus, for larger values of λ_2 the tumor does not grow outward very much, while for small values the tumor diffuses more and gains a larger area.