Faculty of Electrical Eng, Mathematics and Computer Science

Lab Assignment 6B
WI4243FEM
Finite-element analysis for Applied Physics

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1 Problem Statement

We consider a circular slab of an infected organic fluid where pathogens (bacteria) consume oxygen, where a fluid flow is induced by motion. In this assignment, we only consider the consumption of the oxygen by the pathogens, and the diffusion of the oxygen through the tissue. Far away from the domain, the concentration of the oxygen is equal to the equilibrium in non-infected tissue and therefore, we assume the concentration to be equal to the equilibrium sufficiently far away. Since we are not able to consider an unbounded domain, we consider a circular domain with radius of 1 micrometer that is $\Omega = \{(x, y) \in \mathbb{R}^2 | x^2 + y^2 < 1\}$ with its boundary $\partial\Omega$. The dimensions are given in *micrometers*. In this assignment, we consider a steady-state equilibrium determined by diffusion and regeneration by the cells. The pathogens are treated as *point sinks*. Considering n_{cell} cells, we solve

$$-\nabla \cdot (D\nabla u) + \nabla \cdot (u\mathbf{v}) + \sum_{p=1}^{n_{cell}} Q_p u \delta(\mathbf{x} - \mathbf{x}_p) = 0, \quad (x, y) \in \Omega, \tag{1}$$

where D denotes the diffusion coefficient, $\mathbf{v}$ represents the velocity vector of the gel-like fluid and Q_k denotes the hormon secretion rate by cell k. Here u denotes the oxygen concentration. We use the convention $\mathbf{x} = (x, y)$ to represent the spatial coordinates. Further, $\delta(.)$ represents the Dirac Delta Distribution, which is characterised by

$$\begin{cases} \delta(\mathbf{x}) = 0, & \text{if } \mathbf{x} \neq \mathbf{0}, \\ \displaystyle\int_\Omega \delta(\mathbf{x}) d\Omega = 1, & \text{where } \Omega \text{ contains the origin.} \end{cases} \tag{2}$$

Next to the above partial differential equation, we consider the boundary condition

$$D\frac{\partial u}{\partial n} - \mathbf{v} \cdot \mathbf{n} u + K(u - u^\infty) = 0, \quad (x, y) \in \partial\Omega. \tag{3}$$

Here K denotes the transfer rate coefficient of the hormon between the boundary of the domain and its surroundings. For the computations, we use the following values:

Table 1: Values of input parameters

Symbol	Value	Unit
D	$2.3 \cdot 10^{-1}$	$\mu m^2/s$
Q_p	$1 \cdot 10^{-1}$	$1/s$
K	10	$\mu m/s$
u^∞	1	mol
v_x	$\frac{10}{\sqrt{2}}$	$\mu m/s$
v_y	$\frac{5}{\sqrt{2}}$	$\mu m/s$

We consider five cells, located at

$$\begin{cases} x_p = 0.6\cos(\dfrac{2\pi(p-1)}{5}), \\ \\ x_p = 0.6\sin(\dfrac{2\pi(p-1)}{5}), \end{cases}$$

$p \in \{1, \ldots, 5\}$. In order to solve this problem, one needs to consider the following questions:

1. Give the weak formulation of the problem (partial differential equation + boundary condition). *Hint:* $\int_\Omega \delta(\mathbf{x}) f(\mathbf{x}) d\Omega = f(\mathbf{0})$.

2. Give the Galerkin equations (the system of linear equations).

3. Give the element matrix and element vector for the internal elements. Distinguish between cases where the point sink lies inside or outside the considered element.

4. Give the element matrix and element vector for the boundary elements.

5. In order to solve the problem, you need to determine whether each internal element (triangle) contains a cell. We will determine whether cell with index p, with position $\mathbf{x}_p$, is in the element e_k with vertices $\mathbf{x}_{k1}$, $\mathbf{x}_{k2}$ and $\mathbf{x}_{k3}$. We do so by testing the following criterion:

$$|\Delta(\mathbf{x}_p, \mathbf{x}_{k2}, \mathbf{x}_{k3})| + |\Delta(\mathbf{x}_{k1}, \mathbf{x}_p, \mathbf{x}_{k3})| + |\Delta(\mathbf{x}_{k1}, \mathbf{x}_{k2}, \mathbf{x}_p)| : \begin{cases} = |e_k|, & \mathbf{x}_p \in \overline{e}_k \\ \\ > |e_k|, & \mathbf{x}_p \notin \overline{e}_k. \end{cases} \tag{4}$$

   Here $\Delta(\mathbf{x}_p, \mathbf{x}_q, \mathbf{x}_r)$ denotes the triangle with vertices $\mathbf{x}_p$, $\mathbf{x}_q$ and $\mathbf{x}_r$, and $|\Delta(\mathbf{x}_{k1}, \mathbf{x}_{k2}, \mathbf{x}_{k3})|$ denotes its area. Further, $e_k = \Delta(\mathbf{x}_{k1}, \mathbf{x}_{k2}, \mathbf{x}_{k3})$ represents the triangular element k with vertices $\mathbf{x}_{k1}$, $\mathbf{x}_{k2}$ and $\mathbf{x}_{k3}$ and $\overline{e}_k$ includes the boundaries of element e_k. Express the area of the triangles in terms of the nodal points (*Hint: Use the determinant as in Chapter 6 of the book.*). To implement the above criterion whether a cell is within an element, use a tolerance of eps in matlab because of possible rounding errors.

   Remark: As an alternative to the above procedure, you may also consider the barycentric coordinates, which are the linear basis functions ϕ_{k1}, ϕ_{k2} and ϕ_{k3}, and see whether their values are in the interval $[0, 1]$ for $\mathbf{x}_p$, then, $\mathbf{x}_p$ is within the triangular element e_k.

6. Program the finite-element code (GenerateElementMatrix, GenerateElementVector, GenerateBoundaryElementMatrix, GenerateBoundaryElementVector), and evaluate the solution. Use mesh refinement to evaluate the quality of the solution. Plot your solution in terms of contour plot and a three-dimensional surface plot.

7. Perform various simulations where you let the transfer coefficient K range between 0.00001 and 10000. Show the contour plots. Explain your results.

8. Multiply the velocity by 10, what do you observe? How could the solution be improved?