9. Computer Lab 5: Civil Engineering Case Study.

Numerical Computation of the Pollutant Concentration due to a Toxic Spill

- BACKGROUND

It is only recently that humanity has recognized the importance of protecting the environment. Air and water pollution, and their impact on global warming and aquatic life are common subjects of discussion. There exists however another form of pollution, which is as important as air and water pollution: pollution of the soil. Due to toxic spills or the overuse of chemical products in agriculture, soils in many industrialized countries are often found to be unusable, perhaps even dangerous to plant, animal and human life (Sydney tar ponds, NS).

The problem of interest in this lab is at the residential level. We are concerned with a dwelling constructed about 50 years ago and located on a private island. Electrical power is not distributed to the island so a diesel generator is used to produce the necessary electricity. The diesel tank has a capacity of 1000 litres and is buried below the ground level, a few meters away from the house. Unfortunately, at the time tanks were fabricated of steel which erodes over time, so after about 10 years the tank began to leak. The owners being negligent never inspected their tank so the leak was not noticed until they wanted to sell their property, new laws requiring that a dwelling be thoroughly inspected before sale. It was discovered at this time that the diesel had penetrated the soil and diffused right up to the lake surrounding the island. The island must be decontaminated.

The engineering consulting firm hired to decontaminate must first evaluate the quantity and distribution of diesel in the ground. In order to do this the engineers make the following hypotheses:

- The concentration of pollutant at the source of the contaminant (at the tank) is maximal and the soil at this location is saturated with pollutant. The soil is found to be porous by a factor of 0.2, which means that before the spill, the volume of air was 20% of any given volume of soil. The volume concentration of diesel near the tank is thus 200 l/m^3 since the soil is saturated in this location.
- The water from the lake acts as a dilutant so the concentration of pollutant near the edge of the island is negligible (zero).
- The ground forming the island is comprised of about a 1 meter mix of sand, silt and organic material on waterproof clay. The diesel was thus able to infiltrate only the first meter of ground material.
- The ground is roughly the same all over the island.
- The leak has been ongoing for a very long time so the concentration of pollutant in the soil is considered to be at equilibrium. This implies that the source of pollutant has never changed and that the water in the lake has always been at the same level.
- We can also assume that the concentration of pollutant is constant vertically throughout the 1 meter mixture of sand, silt and organic material.

Based on these hypotheses, the concentration of diesel in a 1 meter depth of soil, denoted C in units of l/m^3, can be approximated by the two-dimensional diffusion equation given below (Laplace's equation):

$$\frac{\partial^2 C_{\text{diesel}}}{\partial x^2} + \frac{\partial^2 C_{\text{diesel}}}{\partial y^2} = 0 \qquad (9.1)$$

In order to solve this equation and given the complex geometry of the island, the consulting firm wishes to implement a computer program to solve numerically this equation. One of the simplest methods that can be used to solve this equation is the Gauss-Seidel relaxation method. The method consists in replacing the domain of interest (the island) with a uniform mesh of nodes. At each node, a value of concentration will be computed. The geometry of the island and the mesh of nodes to be used for the analysis are shown in Figure 9.1. Each node corresponds to 10 km^2 of soil surface. The position of the source of pollutant is identified as the large dot. Each node is identified by its row number i and its column number j.

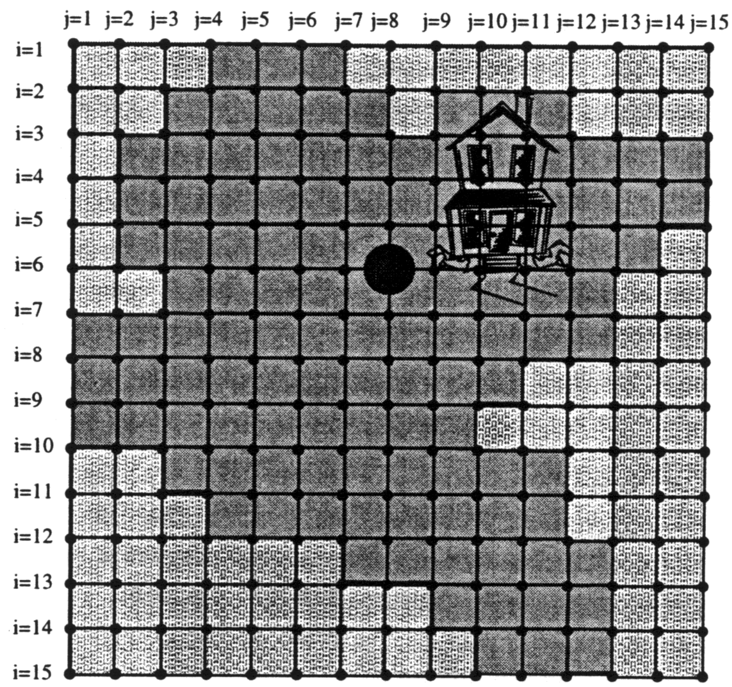

Fig. 9.1: Geometry of the island, position of the source of pollutant and mesh of nodes used for the calculation.

The calculation of the concentration at node (i;j) can be performed using the following equation:

$$C_{\text{diesel}}(i;j) = \frac{C_{\text{diesel}}(i-1;j) + C_{\text{diesel}}(i+1;j) + C_{\text{diesel}}(i;j-1) + C_{\text{diesel}}(i;j+1)}{4} \qquad (9.2)$$

In other words, the concentration at each node is the average value of the concentration at the 4 neighboring nodes (Figure 9.2).

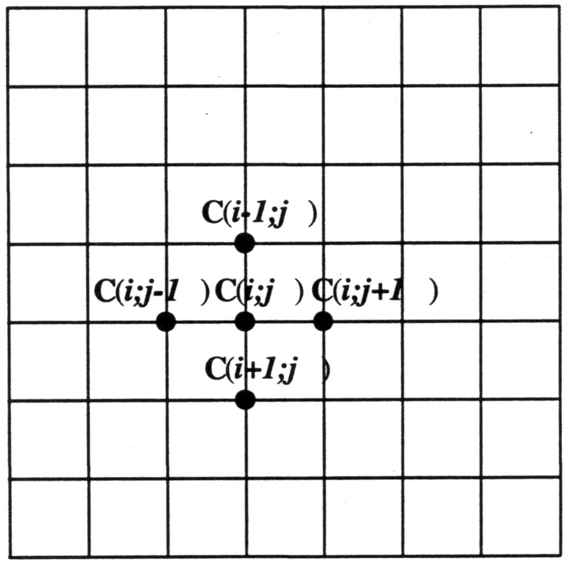

Fig. 9.2: Schematic representation of the nodes used in the relation method.

To compute the concentration at every node we proceed as follows:

- Begin with a series of initial values at every node; the initial values are taken as zero everywhere except at the source node (location of the tank).
- We then update the concentration at each node using equation (9.2).
- Numerous iterations (or updates) over the entire computation domain (each node) are required for the solution at all nodes to approach the exact solution to equation 9.1
- After each iteration the new concentration at each node tends towards the exact concentration.

To determine if another iteration is necessary, we must define a convergence criterion. This criterion should allow us to assess whether our numerical solution is accurate enough to be taken as the real solution over all nodes. Our criterion is based on the variation of the concentration values at all nodes between the previous iteration m-*1* and the present iteration m. This variation is written as:

$$\Delta C^{(m)} = \text{abs}(C^{(m)} - C^{(m-1)}) \qquad (9.3)$$

where C^{m-1} is the value of the concentration at the previous iteration.

Our convergence criterion is the following:

$$\left(\frac{\Delta C^{(m)}}{C^{(m)}}\right)_{\max} < accuracy \qquad (9.4)$$

where *accuracy* is a value of the desired accuracy (often taken as 1×10^{-4}). This convergence criterion is used to determine when to stop the iterations. It means quite simply that we are to stop iterating when the largest variation over all nodes is inferior to the requested accuracy.

Not all nodes take part in the iterative calculation. The nodes located in the water for example always have a zero concentration of pollutant. The nodes located on the water-island boundary also always have a zero concentration. Finally the node that corresponds to the source of pollutant (tank) has a constant concentration of 200 l/m^3 during the entire calculation time.

Once the concentration of pollutant all over the island has been found, we can proceed with the computation of the total quantity of pollutant Q in liters in the ground using the following approximation:

$$Q = \sum_i \sum_j hAC(i;j) \qquad (9.5)$$

where h is the depth of the contamination ($h=1m$), A is the area of the soil at each node, and C(i;j) are the final values of concentration obtained from the iterative calculation procedure.

- ASSIGNMENT

This assignment consists in developing the three functions used by the **main()** program provided. The data describing the horizontal geometry of the problem are given in the ASCII file **island.txt**. Both this file and the main() module can be downloaded from the course Website.

The file **`island.txt`** must be placed in an appropriate directory on the system used to perform the calculations. The file contains the following information:

- On the first line, two integers are given corresponding to the number of rows **`nrows`** and the number of columns **`ncols`**, respectively.
- A 2-D array of size **`nrows`** × **`ncols`** is then given. This is an array of integers comprised of the values 0 or 1 indicating which nodes take part in the calculation process. If the code is 0 then the node at the corresponding position does not take part in the calculation process and the concentration value at the node remains constant at the initial value. If the integer is 1 then the node does take part in the calculation process and the concentration at the node is computed using equation (9.2).
- Finally, a 2-D array of size **`nrows`** × **`ncols`** is given in the file. This is an array of real numbers that are the initial concentration values to be used for the corresponding nodes.

The main program calls the three functions that you must create. Be sure to adhere to the prototypes given in **`main()`** for each of the functions. Also consult these prototypes to determine the I/O required for each function. Each function must perform the following tasks:

<u>1. Data entry function:</u>

- Prompts the user for the name of the data file.
- Reads in the data contained in the file, ensuring that the amount of data read fits into the arrays declared.
- Returns to the caller the data read via the argument list.
- The function must return to the caller the integer 1 if no errors were encountered during the reading of the file or 0 if a reading error occurred.

<u>2. Function to compute the concentrations:</u>

- Executes the iterative computation of the concentration at the required nodes using Eq. (9.2).
- After each iteration, the value of $(\Delta C^m / C^m)_{max}$ must be computed and printed to the screen along with the iteration number so that the user can follow the evolution of the computations. The convergence criterion as given by Equation (9.4) must be evaluated after each iteration in order to determine if another iteration is to take place. A maximum limit for the number of iterations must also be placed so that the iterations eventially end in the event of non-convergence of the results.
- The function returns to the caller the array of results passed in as an argument of the function.
- The function returns to the caller the integer 1 if convergence has been achieved or the integer 0 if the results have not converged.

<u>3. Function to Compute the Total Quantity of Pollutant</u>

- This function returns to the caller the total quantity of pollutant computed using Equation (9.5).

Depending on the value used to assess the accuracy of the concentration in Equation (9.4), the total quantity of pollutant Q, computed via Equation (9.5) can vary greatly. Vary the accuracy parameter in Equation (9.4), using the values 1.0×10^{-3}, 1.0×10^{-4} and 1.0×10^{-6}, and give the associated number of iterations required to complete the calculation and the resulting quantity of total pollutant Q. Discuss these results. Include in your report only one output window for the case where the accuracy takes on the value: 1.0×10^{-3}.