THE UNIVERSITY OF QUEENSLAND

MECH 3750

Part 2 -- PDE;

Assignment 2

Engineering Investigation

2018

A. Investigation problem

(the problem to be solved and presented in the submission)

After an accident, some amount of a pollutant was spilled into environment. The accident has not been noticed and pollutant concentration f diffused according to the equation

(1) $$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}$$

for some unknown time. The properties of the media are known, and as such the diffusion coefficient, $\boldsymbol{D} = \mathbf{0.5}\boldsymbol{m^2/day}$. The pollutant was spilt near a river with a 14m section extending from its bank. As such, we can treat the domain as extending from $\boldsymbol{x} = \mathbf{0}$ where an impervious wall is situated (i.e. no pollutant can flow out of this boundary) to $\boldsymbol{x} = \mathbf{14}$ at the river edge (where the pollutant is washed out into the environment, i.e. the quantity of pollutant at this location is $\mathbf{0}$). Therefore, we can treat this problem in one spatial dimension over the domain $\boldsymbol{x} = [\mathbf{0}, \mathbf{14}]$ and the environmental conditions give us the boundary conditions:

(2) $$\frac{\partial f}{\partial x} = 0 \text{ at } x = 0$$

(3) $$f = 0 \quad \text{at} \quad x = x_b = 14m$$

for all times t. When the accident was noticed, measurements were conducted and concentration of the pollutant $f_1(x_i)$ was determined at a series of locations x_i (these data in kg/m are supplied in a separate file).

The overall amount Q of the pollutant spilt is defined by the integral

(4) $$Q = \int_0^{x_b} f dx$$

It is your job to (i) Estimate the time that the spill started leaking into the river, t_s (relative to the time of the measurement) and (ii) determine the amount of the pollutant that was washed away i.e. $\Delta Q = Q_0 - Q$ where Q_0 is the amount spilt and Q is the total amount of the pollutant at the time of the measurement. Give at least 8 digits for your estimate of the value ΔQ and at least 4 digits for t_s.

Important:

- It is known that at the time of the spill, the pollutant was not present near the river (i.e. the pollutant was not leaking into environment);
- Please see Section E for a breakdown of what needs to be submitted and the marks associated with each section of this assignment;
- There is an Auxiliary question in Section C that will help you approach the problem detailed above. This is worth marks in the assignment, and it is strongly recommended that you complete this prior to starting the investigation.

B. Hints

General: This is an ill-posed problem, which requires solution of the diffusion equation back in time. These are most difficult problems that cannot be solved by most conventional methods. We recommend to use separation of variables and restrict the number of harmonics. Too many would cause instability, too few would make the solution inaccurate. Note that you can find only an approximate solution for this problem. You need to find a solution that becomes localised away from the right boundary. Also note that the physical *f* is non-negative.

Separation of variables

Expand $f(x,t) = \sum_k \varphi^{(n)}(t) g^{(n)}(x)$ with $g^{(n)}(x) = \cos(k_n x)$ where k_n, n=1,2,3,... is to be determined from the boundary conditions and $\varphi^{(n)}(t)$ is to be found from substitution to the diffusion equation. Note that k_n, must be different from the values used to solve in tutorial problems due to the Neumann boundary condition in eq (2).

Integrals

Use a discrete representation for all integrals involved using N=71 grid points from x_0=0m to x_{71}=14m spaced by Δx=0.2m. When evaluate the integrals and dot-products, use the trapezoidal rule, that is

(5) $$Q = \int_0^{x_b} f dx = \Delta x \left(\sum_{j=1}^{N-1} f_j + \frac{f_0 + f_N}{2} \right)$$

And for the inner (dot) product of two functions, say $g^{(a)}(x)$ and $g^{(b)}(x)$

(6) $$\left(g^{(a)}(x) \bullet g^{(b)}(x) \right) = \frac{2}{N} \left(\sum_{j=1}^{N-1} g_j^{(a)} g_j^{(b)} + \frac{g_0^{(a)} g_0^{(b)} + g_N^{(a)} g_N^{(b)}}{2} \right), \qquad \text{where } g_j^{(n)} = g^{(n)}(x_j)$$

Expansion

When using spectral methods, you need to expand the given function $F_0(x)$ (i.e. the initial condition: $F_0(x) = f(x)$ at t=0) into a series

(7) $$F_0(x_j) = \sum_n A_n g^{(n)}(x_j), \quad n = 1,2,..., \quad j = 0,1,...,N$$

You have learned these expansions in **Part 1** of this course: for orthogonal functions $g^{(n)}$

(8) $$A_n = \frac{\left(g^{(n)} \bullet f \right)}{\left(g^{(n)} \bullet g^{(n)} \right)}$$

Note: you must check orthogonality: $\left(g^{(a)} \bullet g^{(b)} \right) = 0$ for any $a \neq b$

C. Auxiliary problem

The auxiliary problem is suggested to code and test numerical schemes for solving the diffusion equation. This is the first step in solving the main investigation problem.

Consider the following auxiliary problem to be solved forward in time

1) $$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}$$

The diffusion coefficient is $\boldsymbol{D = 0.5 m^2/day}$. The boundary conditions are

(2) $$\frac{\partial f}{\partial x} = 0 \text{ at } x = 0$$

(3) $$f = 0 \quad \text{at} \quad x = x_b = 14m$$

The initial conditions f=F_0(x) at time t=0 are provided in the separate file. Obtain solution f(x) in 2 days from the initial moment

This problem has the same equations (1)-(3) as the investigation problem but is to be solved forward in time (from t=0 to t=2) and has a different initial condition.

D. Instructions

Auxiliary problem:

1. **Download** the initial data $F_0(x)$ from electronic file (data 1).
2. **Finite difference:** solve the auxiliary problem by a finite difference method using 71 grid points (including boundaries). Use explicit, implicit and Crank-Nicolson schemes with CFL numbers of c={1.4,1/2,1}.
3. **Spectral:** Solve the same problem by separation of variables:
   a. Separate variables for eq(1)
   b. select a system of orthogonal functions that satisfies the boundary conditions (2 and 3)
   c. demonstrate orthogonality of these functions
   d. expand function $F_0(x)$ into a series of these functions (by determining numerically the projection coefficients) and check your expansion (show a plot) Indicate how many terms should be used in the expansion.
   e. obtain the solution of the auxiliary problem (show a plot)
4. **Test**: Compare the exact (i.e. spectral) solution at t=2days with the results previously obtained by finite differences (see item 2). Evaluate and report numerical errors of the finite difference solutions (9 values) evaluated as

$$E = \max_j \left| f_j^{\text{f.d.}} - f_j^{\text{exact}} \right|$$

Investigation problem:

1. **Download** the concentrations of the pollutant from the electronic file (data 2).
2. **Check** if you can solve this problem by using finite differences back in time.
3. **Solve** the problem by the spectral method
4. **Restrict** the number of harmonics until a reasonable solution can be obtained for a sufficient time interval back in time until the pollutant separates from the right boundary
5. **Check** that solving forward in time by the Crank-Nicolson finite difference scheme from the function you obtained does produce the given distribution
6. **Evaluate** the initial and the final amounts of the pollutant using equation (4) and obtain ΔQ **(comment** on conservative properties of this equation**)**

E. What to submit? / marking scheme

Summary

- Separation of variables solution for the diffusion equation given;
- Solution to Auxiliary problem
- Solution to the Investigation problem
- Comments & conclusions.

1. **Solution** by separation of variables for this problem no more than 1 page (20 %),
2. For the auxiliary problem (20%):
    a. **Key results** 1: numerical formulation and 3x3 table of evaluated errors E
    b. **Figure 1.** show a) the initial conditions and its spectral approximation b) solution by finite difference scheme (all which are visibly different) and the spectral solution at t=2days
3. For the engineering investigation problem (30%):
    a. **Key results 2**
        i. the integral values Q and Q_0 and your answer for ΔQ; Give no less 8 digits for your evaluation of these values
        ii. the number of harmonics you use to obtain the solution
        iii. the time of the spill (i.e. for how long your solution goes back in time) – at least 4 digits
        iv. The initial distribution evaluated by you
    b. **Figure 2:** plot a) the final distribution (which is given) and the initial distribution that you evaluated by solving back in time
4. **Comments / conclusions** (around 1 page, 30%):
    a. Specification and justification of the choices you have made and the outcomes
    b. difficulties you had and the way you overcame them
    c. any other comments you wish to make
    d. conclusions: validity and reliability of your results
5. **Your code in python** (compulsory – you must submit your working code for both the auxiliary and investigation problems, although we do not assess its quality independently of your results as long as the code is original and working)

Submission: You will receive instructions for the submission procedure from the senior tutor – please submit accordingly and before to the due date

Note. Ill-posed problems are the hardest possible types of problems that can be solved only by a very limited group of methods. Some of you may fail to obtain a reasonable solution. In this case submit items 1,2,4 and 5 and you will still get (partial) marks for these parts.

Important. The University of Queensland has strict policies against plagiarism. It is utmost important that you follow the rules. Your submission must be strictly individual. Python code: you can use/modify the course sample files but you cannot use any other source, especially any work of the other students. You can consult tutors and other students but the solution and submission must be yours and only yours. You must not reveal to other students (or ask other students to reveal) the exact values of the key results. The comments/conclusion text does not need to be extensive but it must be written by you and reflect your experience in solving this problem.