Maths and Numerical Methods Coursework

Due: Friday 24th January at 12pm for group component submission and 5pm for individual component submission

After the 12pm group component submission a model answer for the code for question 2 will be released for those who wish to use it in the individual component

Note that this coursework counts 1/2 of the total mark for the Maths and Numerical Methods module, with the other 1/2 being based on the class test sat on Thursday 16th January.

The coursework consists of 2 questions, both of which must be answered. Each question must be answered in a separate file. Question one is worth 30% of the total mark for this coursework and question 2 is worth 70%.

Each question will have a group component and an individual component. Overall the group component will be worth 65% of the total mark and the individual component worth 35% of the total mark.

Each group will have a group GitHub repository to which the group solutions must be submitted. In addition, individual submissions must be submitted to the individual GitHub repositories which you will be assigned. Note that there must be no collaboration, even within your group, on these individual submission components and we will be checking for plagiarism.

Question 1

The wave equation for a variable a(t, x) has a canonical form

$$\frac{\partial^2 a}{\partial t^2} = c^2 \frac{\partial^2 a}{\partial x^2}.$$

By splitting the second order PDE into two first order PDEs and replacing the pure time derivative with a material derivative (i.e. advection) and adding diffusion terms and a constant forcing, we obtain the following system:

Forced advected wave equations (FWE)

$$\frac{\partial a}{\partial t} = -U\frac{\partial a}{\partial x} + \kappa_1 \frac{\partial^2 a}{\partial x^2} + b,$$

$$\frac{\partial b}{\partial t} = -U\frac{\partial b}{\partial x} + \kappa_2 \frac{\partial^2 b}{\partial x^2} + c^2 \frac{\partial^2 a}{\partial x^2} + F$$

Where $b(x, t)$ is our supplementary variable connected to the material rate of change of a, U is our constant velocity, κ_1 and κ_2 our diffusivities and F(x) a time-constant forcing function.

For $\kappa_1 = \kappa_2 = 0$, F=0 this system has purely translating solutions of the form

$$a(t, x) = A(x - (U - c)t) + B(x - (U + c)t)$$

$$b(t, x) = (c\text{-U})A'(x - (U - c)t)\text{-}(U + c)B'(x - (U + c)t)$$

for functions A(x) & B(x).

You will find a Python code (based on the code from the PDE lectures) in FTCS_wave_equation.ipynb to solve this numerically using forward time (i.e. forward Euler) and centred space (for the advection, wave and diffusion terms) in a periodic domain [0, L) and plots the results, along with certain non-dimensional numbers from the lectures

Group Component

a) Identify a complete set of non-dimensional groups for the FWE system given above. Consider both the continuous system written above and the discretized system implemented in the notebook we have given you.

   For each discretised non-dimensional group, try to identify any stability criteria you believe relates to it (you may want to pick out quantities which correspond to those given for the advection-diffusion equation in the lecture notes).

   You can provide evidence for your stability hypothesis either experimentally via examples using the code (try to include plots/graphs), or by mathematical analysis or ideally, mixing both. This work should go into the Q1a notebook in your group repository.

(15 marks)

Individual Component:

b) Following the work shown and discussed in the lectures, there are several alternative approaches to discretisation which could be considered:
   I. Switching the space discretization for advection to use upwinding for advection;

II. Changing the time-stepping scheme to an implicit one;
III. Changing the time scheme to a multistep method;
IV. Modifying the equation by adding additional non-physical terms, or removing those which are (e.g. adding extra diffusion, or dropping one of the advection terms).
V. Taking an alternative approach to generating the original system (for example by starting with $c\frac{\partial B}{\partial x} = \frac{\partial a}{\partial t}$, rather than $b = \frac{\partial a}{\partial t}$ when converting the wave equation to first order

Each member of the group should choose a different one of the approaches above and write a short (about 500 to 750 words, or 3 to 6 paragraphs) discussion covering the advantages and disadvantages of that particular approach, considering the effect of changes in the relative magnitude of your various non-dimensional groups from part (a). Team members should not both choose the same approach to write about, and such answers may be penalised. This work should go into the Q1b notebook in your individual repository

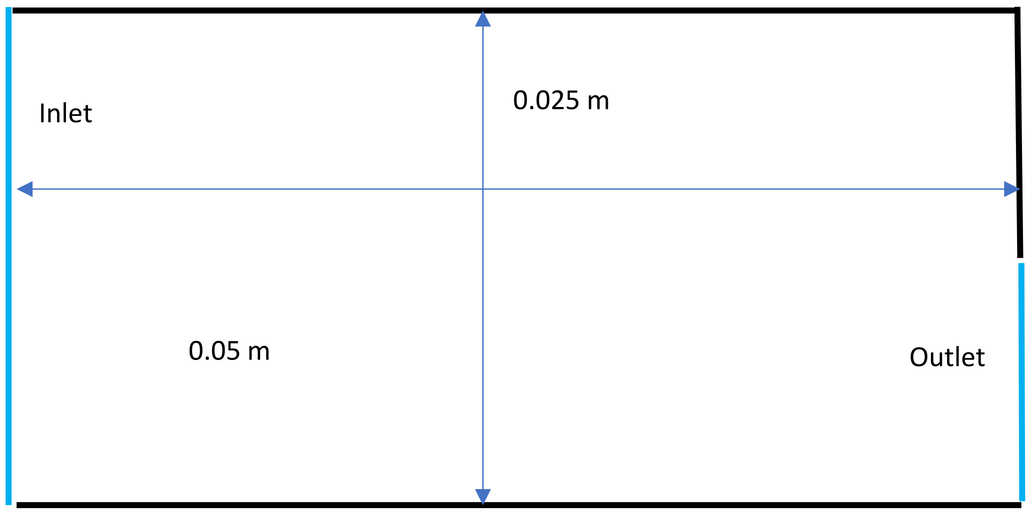
You may include mathematics, numerical Python code implementing methods, images or plots to represent or explain your findings, these will not contribute to your word count.

For both sections more marks will be given for answers that synthesise (i.e. combine and build upon) knowledge from lectures and include your own interpretations and work. You can use any material from lectures or homework, but you are unlikely to score highly simply by copying large chunks of material without demonstrating your own understanding.

In part (b) rather than trying to cover every possible topic, higher marks will be given for a “deep dive” into one particular aspect each for both advantages and disadvantages, e.g. accuracy, generalisability, computational efficiency, stability, underpinning theory, etc. At the start of your answer, give a short explanation for which aspects you have decided to focus on, and how your answer synthesises or expands upon material from the lectures.

[15 marks]

Question 2



A company is designing a reactor to break down pollutants in a liquid stream. The reactor is to consist of two parallel plates with flow between then. In order to enhance mixing the outlet will be the bottom half of the right hand side of the reactor, while the inlet will cover the entire left hand side. All other boundaries can be considered to be no slip.

The fluid properties are those of water ($\rho = 1000\ kg/m^3$ and $\mu = 0.001\ Pa.s$ – note be careful as to which viscosity is being used in the code – $\nu = \mu/\rho$). The pressure drop between the inlet and outlet is 0.5 Pa, with a constant pressure across each of these boundaries.

Group Component

a) Code a simulator to solve this problem. You may modify the code that was developed in class. Show the flow and pressure profiles for the conditions given above. Remember to check if the flow has achieved steady state before plotting the results. (20 marks)

The flow of the contaminant within the water can be described using an advection-diffusion equation with a first order pollutant reaction rate:

$$\frac{\partial C}{\partial t} = -\mathbf{v} \cdot \nabla C + D\nabla^2 C - kC$$

Where C is the pollutant concentration, $\mathbf{v}$ is the liquid velocity vector, D is the diffusivity and k is rate constant. The pollutant concentration at the inlet is 1 kg/m^3, while at the outlet the pollutant flows at the same rate as the fluid, which implies that there is zero gradient in the concentration normal to this boundary. All other boundaries have no flux through them. As there is no flux of liquid through these boundaries as well, this implies that the concentration gradient in the direction normal to these boundaries is also zero. You can use a diffusivity of 1×10^{-6} m^2/s (note that this is quite high compared to the real diffusivities of chemicals in water, but results in Peclet numbers that are likely to produce more interesting results). For the first order reaction rate you can use a value of 0.25 s^{-1}.

b) Write out a finite difference approximation for the advection diffusion equation given above. You can use an explicit scheme (spatial derivatives calculated at the current time step and time derivate between the current and next time step). You must use upwind approximations for the advection terms (don't assume a sign for the fluid velocities – leave them as conditions both in the derivation and the subsequent code). Note that this scheme is similar to what was derived in the lecture on Dimensional Analysis, but with two spatial dimensions rather than one and the inclusion of a reaction term. (10 marks)

c) Implement this approximation together with appropriate boundary conditions within the fluid flow simulator. This therefore takes the form of an initial value problem. In addition to the Courant number stability criterion that should already be applied for the fluid calculations, there is an additional criterion based on the diffusivity – namely that $\Delta t \ll \frac{\Delta x^2}{2D}$. Plot the results of the simulations for the base case conditions given above. What is the average outflow concentration (use the average of point outflow concentration multiplied by the point outflow velocity divided by the average outflow velocity)? Remember to run the simulation until the point at which it approaches steady state in terms of both the flow and the concentration. (20 marks)

Individual Component

d) Numerically investigate how the parameters in the models influence the results (hint: doing this in terms of dimensionless groups may help the analysis). Show trends and discuss the results. (20 marks)