Programming Assignment - 2

In this assignment, your final objective is to numerically solve the unsteady 2-D linear advection-diffusion equation. Along the way, you will implement a multi-step time integration scheme, and the convective schemes studied in class. The governing PDE for the time interval $(0, T)$ in a domain Ω is given by,

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} = \alpha\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) \quad \text{in} \quad (0,T)\times\Omega, \tag{1}$$

$$\phi(x,y,0) = f(x,y), \tag{2}$$

$$\phi = \phi_0 \quad \text{on} \quad \partial\Omega_D, \tag{3}$$

$$\frac{\partial \phi}{\partial n} = g \quad \text{on} \quad \partial\Omega_N, \tag{4}$$

where $\partial\Omega_D$ and $\partial\Omega_N$ denote the regions of the boundary over which Dirichlet and Neumann boundary conditions are applied respectively. u and v denote the velocity field over the domain Ω. The final objective can be achieved by solving the following sub-problems.

1 Unsteady Advection Equation

In this section, you will numerically solve the unsteady Linear Advection equation using explicit time integration methods, by simulating a popular rotating cone CFD benchmark problem. The specific problem is given by

$$\begin{aligned}
\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} &= 0 \quad \text{in} \quad (0,T)\times\Omega = (-1,1)\times(-1,1),\\
\phi(x,y,0) &= 5.0\exp(-1500((x-0.25)^2+y^2)),\\
\phi(x,y,t) &= \phi(x,y,0) \quad \text{on} \quad \partial\Omega,\\
T &= 2\pi,\\
u &= y, \qquad v = -x.
\end{aligned}$$

For the problem, your tasks are as follows:

1. Exact solution
   (a) Consider 1D advection equation $\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0$. How to classify it? How the solution behaves for this class of PDE?
   (b) Plot the initial contour of ϕ and velocity vector (u, v) with Matlab. Then convert the velocity vector from Cartesian coordinate system (u, v) to polar coordinate system (v_r, v_θ). Together with the answer of 1(a), can you write down the exact solution of the current problem?

2. First-order spatial and temporal discretization

   (a) Write down the first-order upwind discretization for the convection term. Complete the corresponding function which takes the solution vector ϕ and calculate the vector $-u\frac{\partial \phi}{\partial x} - v\frac{\partial \phi}{\partial y}$

   (b) Use the forward Euler method to perform time integration. Calculate the solution at $t = 2\pi$ with an isotropic Cartesian grid $\Delta x = \Delta y = h$, with 201 grid points along each direction. What is the largest possible time step you can use? Report the CFL number. (Take convective velocity as c=1).

       Hint: Reference solution for CFL=0.2: $\phi_{\text{max}} = 1.75e - 1, \phi_{\text{min}} = 0$.

   (c) Plot the contour of ϕ. (It is fine as long as you get a cone at the same location. The cone will be dissipated A LOT.)

3. Higher-order discretization

   (a) Discretize the convection term with 2^{nd} order upwind scheme. For the points close to the boundary, use the central difference method.

   (b) Use second order Adams-Bashforth method (AB2, see handout 1) for time integration. Calculate the solution at $t = 2\pi$ with an isotropic Cartesian grid $\Delta x = \Delta y = h$, with 201 grid points along each direction. What is the largest possible time step you can use? Report the CFL number.

       Hint: Reference solution for CFL=0.05: $\phi_{\text{max}} = 1.18, \phi_{\text{min}} = -3.69e - 1$.

   (c) Plot the contour of ϕ.

4. Comparison of schemes

   (a) Compare the first order upwind + FE and second order upwind + FE. Which one allows larger Δt? Which one gives you a better solution in terms of accuracy (ϕ_{max} and ϕ_{min})? Plot the contours of ϕ. Which one is more diffusive thus giving less oscillation? Comment based on numerical stability, accuracy and diffusion. (No derivation is needed)

   (b) According to what you learnt from class, comment on the stability of the central difference method for convection + forward Euler for time integration (No derivation is needed). Try the central difference method for convection + AB2. Is it stable or not? What is the largest possible time step you can use? Report the CFL number. Which method you have learnt from class might be helpful for explaining this? Just name one or few and explain why.

2 Unsteady Advection-Diffusion Equation

From section 1, you have constructed a code for applying the discrete Convection operator on a variable defined on Ω. In this section, you will use the ideas developed earlier to solve the unsteady advection-diffusion equation using an Implicit-Explicit approach. Further, you will implement Neumann Boundary Conditions in the current section. The specific problem is given by

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} + v\frac{\partial \phi}{\partial y} = \alpha\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2}\right) \quad \text{in} \quad (0,T)\times\Omega = (0,1)\times(0,1),$$

$$\phi(x,y,0) = 1.0\exp\left(-1500((x-0.5)^2 + (y-0.5)^2)\right), 0 < x < 1, 0 < y < 1$$

$$u(x,y,t) = 1.0,$$

$$v(x,y,t) = 0.05,$$

$$\phi = \begin{cases} 0.1\left(\frac{1-\exp(vy/\alpha)}{1-\exp(v/\alpha)}\right), & x = 0, \quad 0 \le y \le 1, \\ 5.0 + 0.1\left(\frac{1-\exp(vy/\alpha)}{1-\exp(v/\alpha)}\right), & x = 1, \quad 0 \le y \le 1 \end{cases}$$

$$\frac{\partial \phi}{\partial n} = \begin{cases} 0.1\left(\frac{-v}{\alpha(1-\exp(v/\alpha))}\right), & 0 \le x \le 1, \quad y = 0 \\ 0.1\left(\frac{-v\exp(v/\alpha)}{\alpha(1-\exp(v/\alpha))}\right), & 0 \le x \le 1, \quad y = 1. \end{cases}$$

Discretization schemes:

- For the spatial discretization, discretize the convective and diffusive terms using the 2^{nd} order central differencing scheme.
- For the Neumann boundary condition, use first order one-side differentiation to approximate the first order derivative.
- For the time integration, Use (a) Adams Bashforth method for the convective terms and (b) Trapezoidal method for the diffusive terms.

Numerical parameters:

- Use isotropic Cartesian grid $\Delta x = \Delta y = h$ with grids of 17, 65 and 257 grid points along each direction.
- Use $\alpha = 0.1$.
- Note that the initial condition only applies for the interior domain. The initial condition for the boundary is the same with the boundary condition

Your tasks are:

1. Derive the error-residual form. (Hint: this is a linear problem).
2. Determine the largest time step for each grid size. Express your answer as CFL number.
3. Integrate the equation to steady state, when $||\phi^{n+1} - \phi^n||_{L2} < 1e-8$.
   (a) Plot the contours of the steady state solution ϕ. Compare the numerical solution with the exact solution $\phi_e(x,y) = 5.0\left(\frac{1-\exp(ux/\alpha)}{1-\exp(u/\alpha)}\right) + 0.1\left(\frac{1-\exp(vy/\alpha)}{1-\exp(v/\alpha)}\right)$ along the lines $x = 0.5$, $y = x$, and $y = 0.5$. Can you claim convergence of the solution?
   (b) Determine $||\phi - \phi_e||_{L2}$, and show the log-log plot of the L2 norm of error and grid-size. Calculate the slope of the line obtained.
4. Modify $\alpha = 0.0001$ and repeat steps 2. Do you have to modify Δt obtained in step 2?