APC523PS3

Introduction

- Github repository for assignment 4 in APC523 is here: https://github.com/ZINZINBIN/APC523PS4
- Problem 1-(a), Problem 2, Problem 3-(a), and 3-(b) are noted as handwriting. The solution is uploaded via handwriting.pdf.

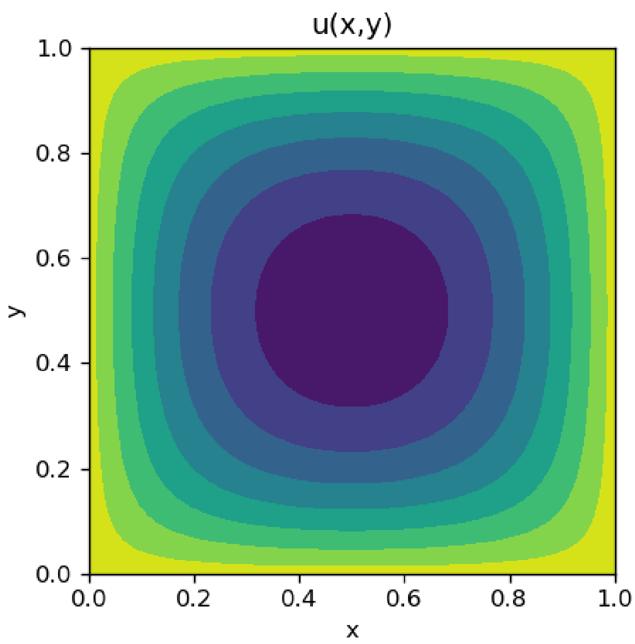
Problem 1. Eliptic BVP

Problem 1.a

The detailed derivation of the reformulation of the BVP in equation (1) as a root-finding problem is noted on handwriting.pdf. Briefly, the laplacian operator is now discretized so that it can be treated as a linear operator. The right hand side of the laplace equation is u^4, Therefore, we can define nonlinear function $g(u) = Lu - u^4$, where $u \in R^{N_{mesh}^2}$. Then, it is allowed to use Newton-Rapson method to compute the root with given Jacobian of $g(u)$.

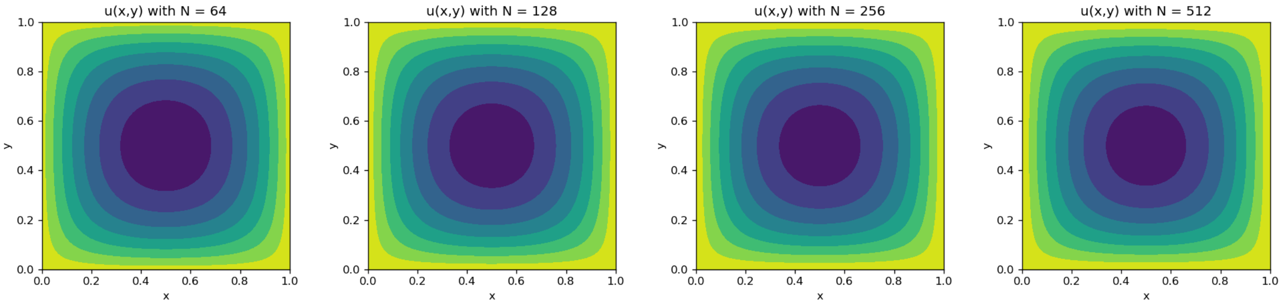
Problem 1.b

In this problem, the Newton-Rapson method with LU decomposition and 5-point second order discretized laplacian is applied. LU decomposition is used to compute the inverse matrix of Jacobian for each step. Considering the Dirichlet boundary condition, we added the boundary value after computing the residual $g(u)$ by $\frac{1}{h^2}$. The numerical result of $u(x,y)$ with directly computing the inverse of Jacobian is given below.

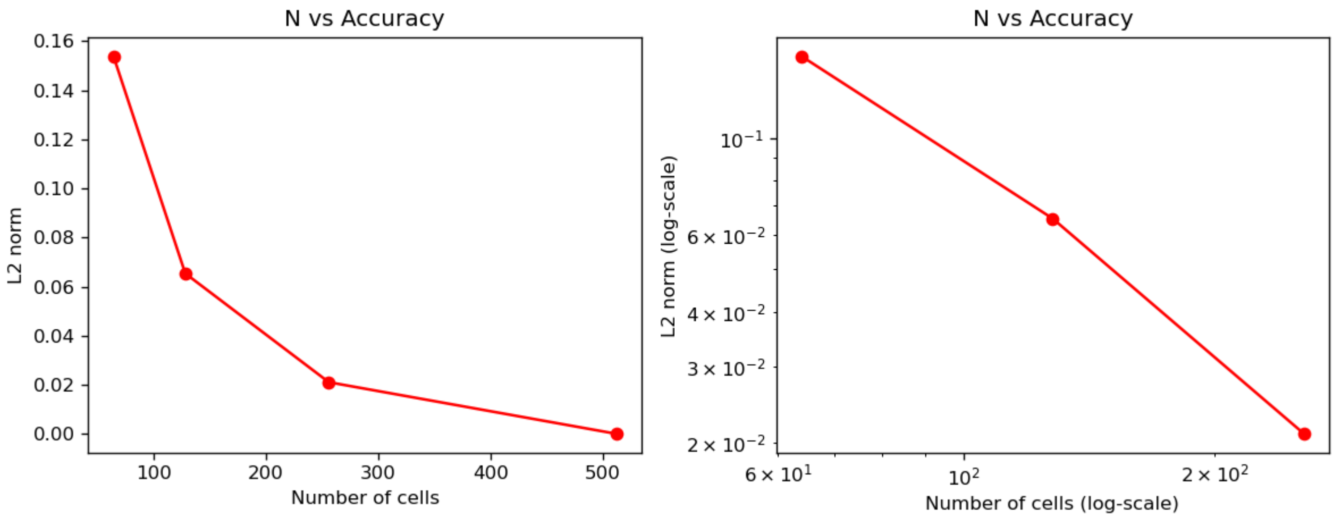


Problem 1.c

As a iterative method to compute the inverse of Jacobian for $g(u)$, weighted Jacobi method was originally utilized and we could observe that this method can also find the solution. However, if the size of the mesh become larger, the computational cost and memory required is also larger so that our resources is not enough then. Therefore, we instead use scipy.sparse matrix and functions with generalized minimal residual iteration to get $J^{-1}g(u)$ direclty from solving $Jx = g(u)$, instead of solving J^{-1} and then multipying $g(u)$. The convergence criteria for computing $J^{-1}g(u)$ is 10^{-8} with $N_{iter} = 16$. Then, all the iterative processes are set as $N_{epoch} = 64$. In this problem, $N_{mesh} = 64, 128, 256$ are given. The below figure shows the contour plot of the solution with different mesh size.



The L2 norm error between the above computed $u(x, y)$ and the ground-truth $u(x, y)$ with $N_{mesh} = 512$ as a function of N_{mesh} is given below. We can observe that the L2 norm error is proportional to $\frac{1}{N^2}$, which can be checked by log-scale graph.



Problem 2. Beam-warming Scheme

The detailed derivation of the modified equation for the Beam-warming scheme is noted on handwriting.pdf. Please see the attached file.

Problem 3. Advection

Problem 3.a and b

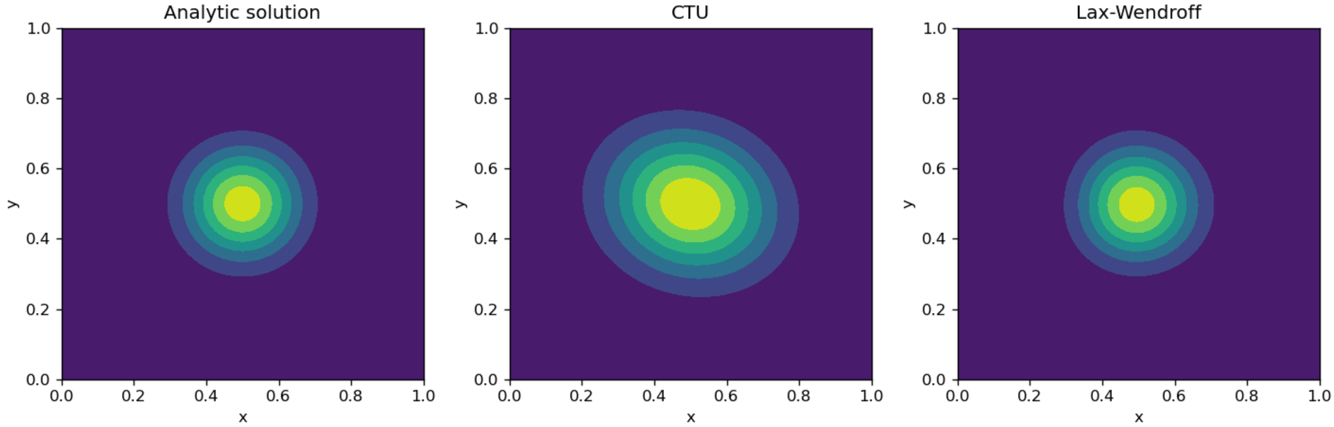
The handwriting solution for proving the analytical solution of $u(t, x, y)$ and the Corner Transport Upstream (CTU) method are derived on handwriting.pdf. Please see the attached file.

Problem 3.c

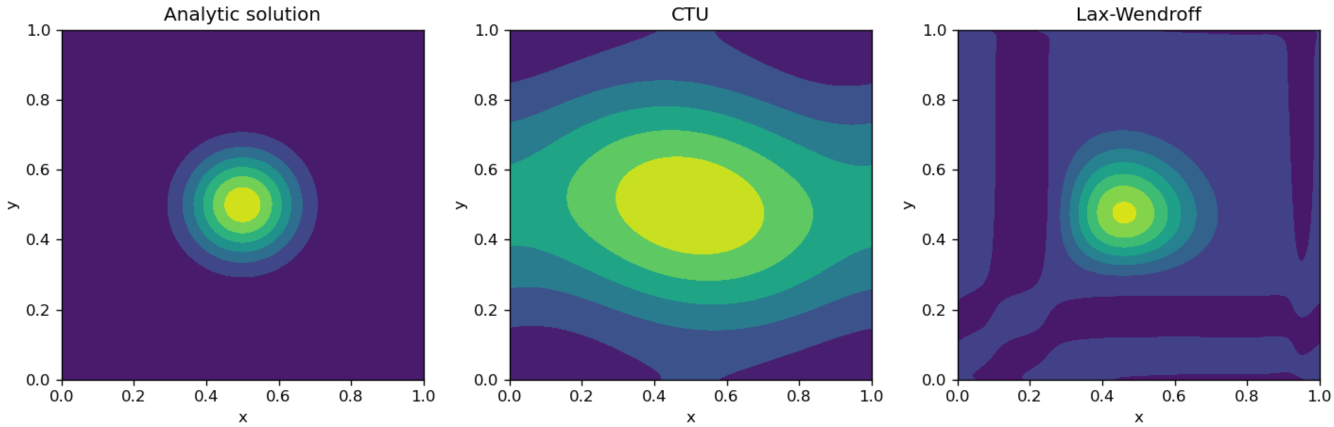
In this problem, CTU and Lax-Wendroff method are implemented based on the equation derived on (b) and (c). The time difference is defined as $dt := \frac{C_{CFL}}{a/dx + b/dy}$ during the simulation to guarantee the numerical stability. The coefficient C_{CFL} is set as 0.4, and other parameters including a, b are set as given in the statement. Following the statement, we plot the contour for each case with different resolutions at $t = 1.0, 10.0$.

The contour plots of $u(t = 1.0, x, y)$ and $u(t = 10.0, x, y)$ with $N = 128$ is given below.

- $u_{128}(t = 1.0, x, y)$

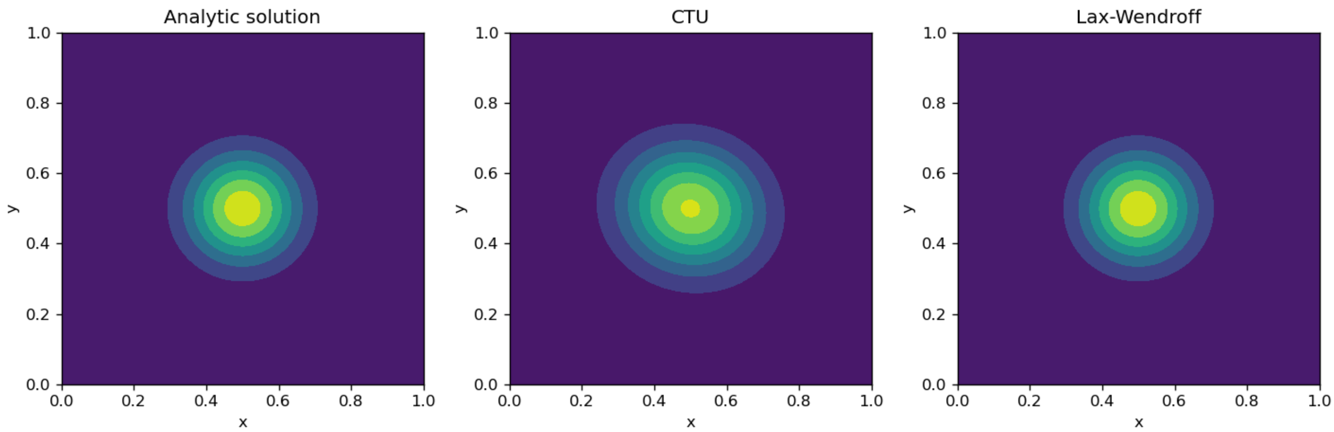


- $u_{128}(t = 10.0, x, y)$

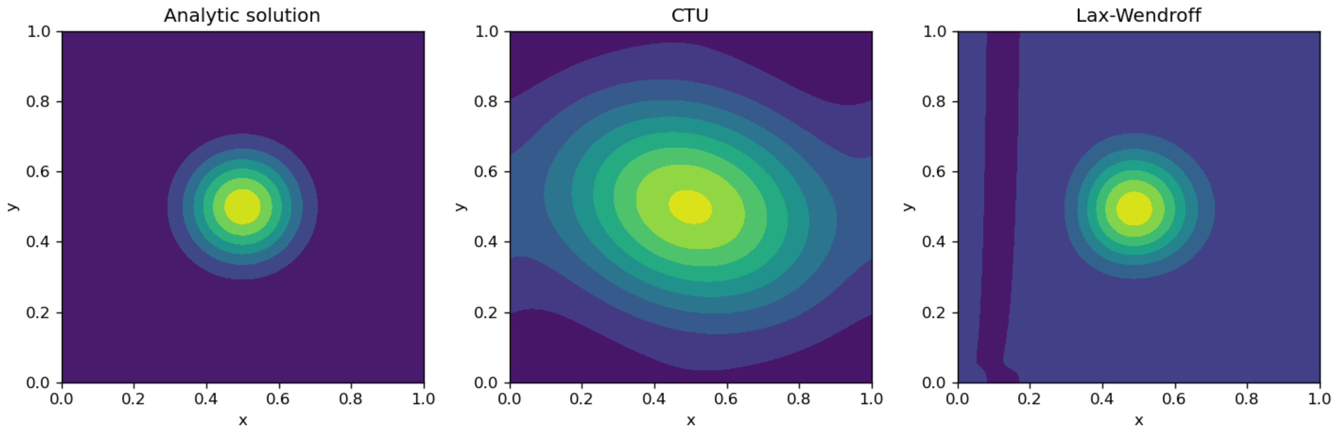


The contour plots of $u(t = 1.0, x, y)$ and $u(t = 10.0, x, y)$ with $N = 256$ is given below.

- $u_{256}(t = 1.0, x, y)$

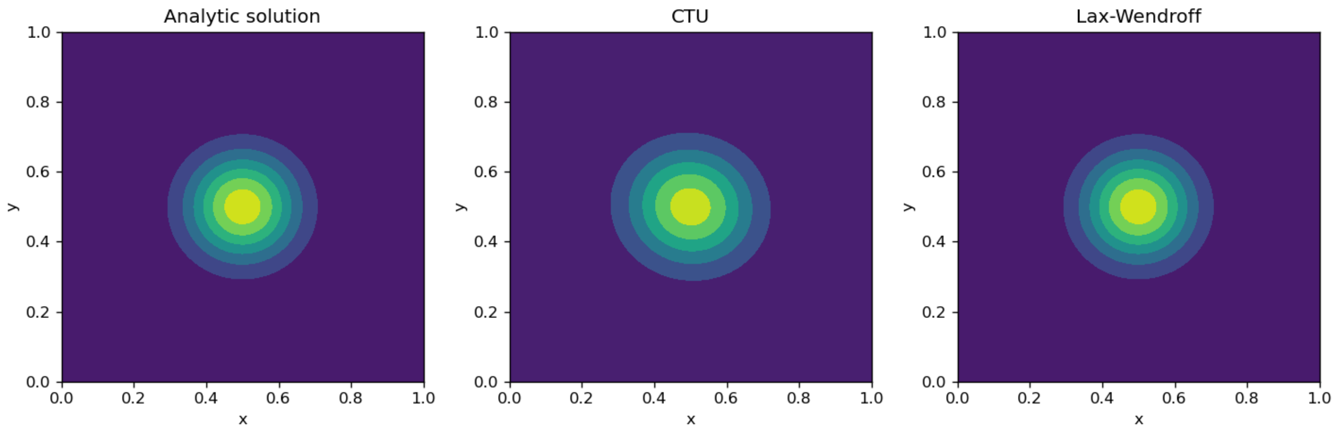


- $u_{256}(t = 10.0, x, y)$

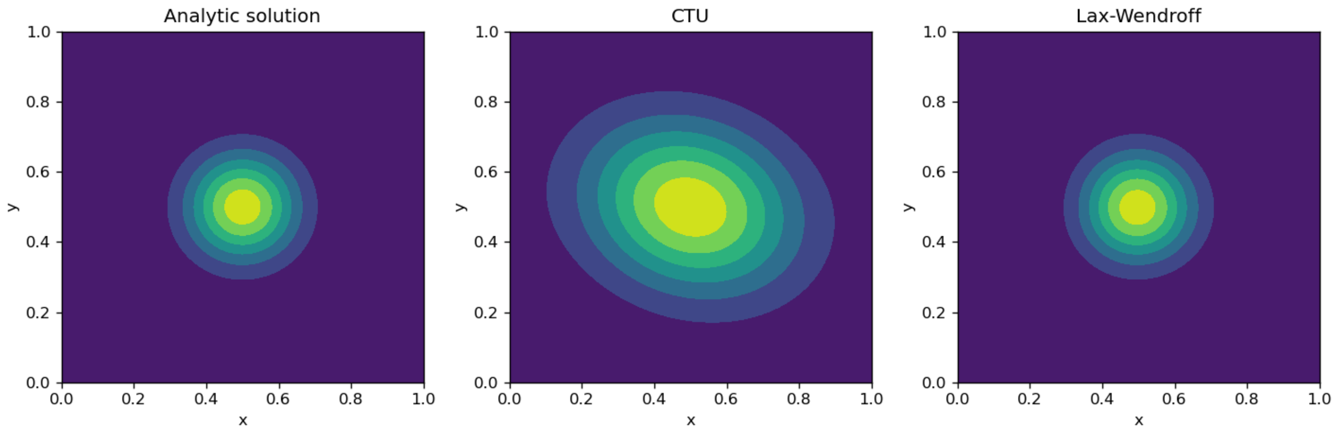


The contour plots of $u(t=1.0,x,y)$ and $u(t=10.0,x,y)$ with $N=512$ is given below.

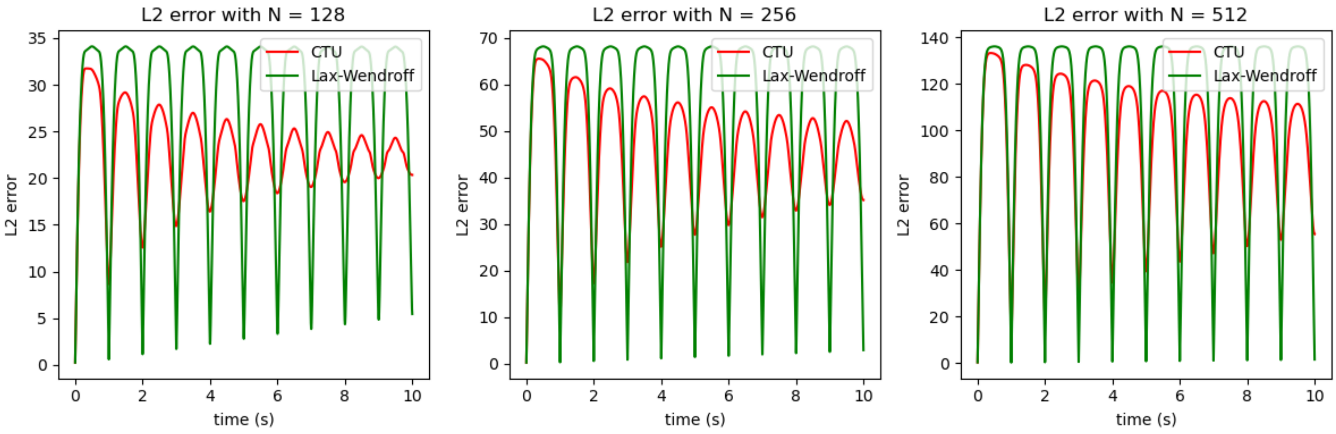
- $u_{512}(t=1.0,x,y)$



- $u_{512}(t=10.0,x,y)$



Lastly, the numerical result for L2 norm of the error as a function of time for $u(t,x,y)$ with different resolutions is given below.


L2 error with N = 128
L2 error with N = 256
L2 error with N = 512
CTU
Lax-Wendroff
L2 error
time (s)

1. Elliptic BVP

Let Ω be the planar domain $[0,1]^2$. Consider the boundary value problem (BVP)

$$\begin{cases} \nabla^2 u - u^4 = 0, \ x \in \Omega, \\ u(x) = 1, \ x \in \partial\Omega. \end{cases} \tag{1}$$

Ω is discretized into $N \times N$ cells. We approximate the Laplace operator using the classical 5-point second-order finite-difference approximation.

(a) Reformulate the boundary value problem (BVP) in equation (1) as a root-finding problem that can be solved using the Newton-Raphson method.

(a) Let $u \in \mathbb{R}^{N \times N}$, $u = \begin{bmatrix} u_{11} & \cdots & u_{1N} \\ \vdots & & \\ u_{N1} & \cdots & u_{NN} \end{bmatrix}$ and u_{1D} is

1-dimensional array of u with $u_{1D} \in \mathbb{R}^{N^2}$ such that

$u_{1D} = \begin{pmatrix} u_{11} \\ \vdots \\ u_{N1} \\ u_{12} \\ \vdots \\ u_{N2} \\ \vdots \end{pmatrix}$ then ∇^2 can be linearlized as 2D Laplacian

operator which is denoted as $L \otimes I + I \otimes L$ where L

is 1-Dimensional discretized laplacian operator. $L, I \in \mathbb{R}^{N \times N}$

Let $\nabla^2 = \tilde{L} = L \otimes I + I \otimes L$

Then, $g(u_{1D}) := \tilde{L} u_{1D} - u_{1D}^4$, which is nonlinear function.

This is equivalent to root-finding problem where

$g(x) = 0$ with $x \in \mathbb{R}^m$ $(m = N^2)$

we can apply Newton-Raphson method to find the solution x^*.

$g(x_{k+1}) = g(x_k) + \frac{\partial g}{\partial x_k} \cdot \delta x_k = g(x_k) + J_g(x_k) \cdot (x_{k+1} - x_k) = 0$

$\Rightarrow \quad x_{k+1} = x_k - J_g^{-1} \cdot g(x_k)$ then we can find the solution !! ^^

2. Beam-warming Scheme

Derive the modified equation for the Beam-warming scheme presented in the lecture on "Hyperbolic PDEs":

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{3u_i^n - 4u_{i-1}^n + u_{i-2}^n}{2h} = \frac{a^2 \Delta t}{2} \frac{u_i^n - 2u_{i-1}^n + u_{i-2}^n}{h^2}. \tag{2}$$

Starting from

$$\frac{\partial}{\partial t} u + a \frac{\partial u}{\partial x} = 0 \quad \text{(Burger's equation)}$$

Let $\frac{\partial}{\partial t} u = \frac{1}{\Delta t}(u_i^{n+1} - u_i^n)$

$$u_i^{n+1} = u_i^n + \Delta t \frac{\partial u}{\partial t} + \frac{1}{2}\Delta t^2 \frac{\partial^2 u}{\partial t^2} + \cdots$$

$\frac{\partial u}{\partial t} = -a\frac{\partial u}{\partial x}$ and $\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2}$ thus

$$u_i^{n+1} \doteq u_i^n - a\Delta t \frac{\partial u}{\partial x} + \frac{1}{2}a^2 \Delta t^2 \frac{\partial^2 u}{\partial x^2}$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{\partial u}{\partial x} = \frac{1}{2}a^2 \Delta t \frac{\partial^2 u}{\partial x^2}$$

Use $\frac{\partial u}{\partial x} \doteq \frac{3u_i^n - 4u_{i-1}^n + u_{i-2}^n}{2h}$ and $\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1}^n - 2u_i^n + u_{i-1}^n}{h^2}$

$$\Rightarrow \frac{1}{\Delta t}(u_i^{n+1} - u_i^n) + a\frac{3u_i^n - 4u_{i-1}^n + u_{i-2}^n}{2h} = \frac{1}{2}a^2\Delta t \cdot \frac{u_{i-1}^n - 2u_i^n + u_{i-1}^n}{h^2}$$

3. Advection

Consider a 2D advection equation for $u(t, x, y)$ given by

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = 0, \tag{3}$$

You are given the initial condition

$$u(0, x, y) = \exp\left(-\frac{(x-1/2)^2 + (y-1/2)^2}{(3/20)^2}\right) \tag{4}$$

and advection speeds $a = 1$ and $b = 2$.

(a) Show that the analytical solution is

$$u(t, x, y) = u(0, x - at, y - bt). \tag{5}$$

(a) $\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = 0$ let $\eta = x - at$ $\xi = y - bt$

and $u = u(\eta, \xi)$ then

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial t} + \frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial t} = -a\frac{\partial u}{\partial \eta} - b\frac{\partial u}{\partial \xi}$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \eta}\frac{\partial \eta}{\partial x} = \frac{\partial u}{\partial \eta} \Rightarrow \frac{\partial}{\partial t}u = -a\frac{\partial u}{\partial x} - b\frac{\partial u}{\partial \xi}$$

$$\frac{\partial u}{\partial y} = \frac{\partial u}{\partial \xi}\frac{\partial \xi}{\partial y} = \frac{\partial u}{\partial \xi}$$

Therefore $u = u(\eta, \xi)$ is a solution of $\frac{\partial}{\partial t}u + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = 0$

and $u(\eta, \xi) = u(0, x - at, y - bt)$.

(b) We will now derive a 2D finite-volume numerical scheme based on this exact solution called the Corner Transport Upstream (CTU) method.

(1) For 1D advection, defining $\mu \equiv a\Delta t/\Delta x$, we can reformulate the first-order upwind scheme using the exact solution for piecewise constant initial conditions, projected back to the initial mesh via conservative integration. Show geometrically (using a simple diagram) that projecting back the exact solution gives you the numerical solution

$$u_i^{n+1} = (1-\mu)u_i^n + \mu u_{i-1}^n \tag{6}$$

(2) Using the same geometrical strategy in 2D, derive the projected values of the exact solution back to the initial grid as a function of $\mu \equiv a\Delta t/\Delta x$ and $\nu \equiv b\Delta t/\Delta y$. This should give you the fully discrete form of the CTU scheme.

(3) Derive the modified equation of this scheme and analyze the leading-order error term.

(1) let $\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$ (1D advection problem)

and $\mu := a\Delta t/\Delta x$. This equation can be reformulated as

1st order upwind scheme by forward euler scheme.

$$\frac{\partial a}{\partial t} \approx (a_i^{n+1} - a_i^n)/\Delta t \qquad \frac{\partial a}{\partial x} \approx \frac{a_i^n - a_{i-1}^n}{\Delta x}$$

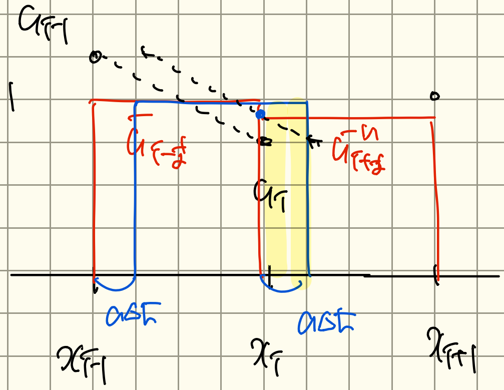
Then $$\frac{\partial a}{\partial t} + a \cdot \frac{\partial a}{\partial x} \approx \frac{1}{\Delta t}(a_i^{n+1} - a_i^n) + a \cdot \frac{1}{\Delta x}(a_i^n - a_{i-1}^n) = 0$$

$$a_i^{n+1} = a_i^n - a\frac{\Delta t}{\Delta x} a_i^n + a\frac{\Delta t}{\Delta x} a_{i-1}^n$$

$$a_i^{n+1} = (1-\mu) a_i^n + \mu a_{i-1}^n$$

This can be shown by geometrical interpretation.

FIG 1



$\frac{\partial a}{\partial t} + a \cdot \frac{\partial a}{\partial x} = 0$: moving flow with a velocity

If Δt time pass, then the amount of moving length is $a\Delta t$

Define $$\bar{a}^n_{i+\frac{1}{2}} = \frac{1}{\Delta x}\int_{x_i}^{x_{i+1}} a(x,t)\,dx$$ then $$\int \left(\frac{\partial a}{\partial t} + a\frac{\partial a}{\partial x}\right) dx\,dt = 0$$

$$\Rightarrow \int_{t_n}^{t_{n+1}} \int_{x_i}^{x_{i+1}} \left(\frac{\partial}{\partial t}a + a\frac{\partial a}{\partial x}\right) dx\,dt = \left(\bar{a}^{n+1}_{i+\frac{1}{2}} - \bar{a}^n_{i+\frac{1}{2}}\right)\Delta x + \Delta t\, a\left(\bar{a}^{n+\frac{1}{2}}_{i+1} - \bar{a}^{n+\frac{1}{2}}_i\right) = 0$$

$$\Rightarrow \bar{a}^{n+1}_{i+\frac{1}{2}} - \bar{a}^n_{i+\frac{1}{2}} + \Delta t \frac{a}{\Delta x} \cdot \left(\bar{a}^{n+\frac{1}{2}}_{i+1} - \bar{a}^{n+\frac{1}{2}}_i\right) = 0$$

Let $i \to i-1$ then this is same as our problem

$$\bar{a}^{n+1}_{i-\frac{1}{2}} - \bar{a}^n_{i-\frac{1}{2}} + \frac{a\Delta t}{\Delta x}\left(\bar{a}^{n+\frac{1}{2}}_i - \bar{a}^{n+\frac{1}{2}}_{i-1}\right) = 0$$

Since the amount of quantities pass at $x = x_i$ is $-a\Delta t\left(\bar{a}^{n+\frac{1}{2}}_i - \bar{a}^{n+\frac{1}{2}}_{i-1}\right)$

this is equal to the change of height $\bar{a}^n_{i-\frac{1}{2}}$ and the

amount is $\left(\bar{a}^{n+1}_{i-\frac{1}{2}} - \bar{a}^n_{i-\frac{1}{2}}\right)\Delta x = -a\Delta t\left(\bar{a}^{n+\frac{1}{2}}_i - \bar{a}^{n+\frac{1}{2}}_{i-1}\right)$

$\Rightarrow$ Thus $(\bar{a}^{n+1}_{i-\frac12} - \bar{a}^{n}_{i-\frac12}) + \mu\,(\bar{a}^{n+\frac12}_{i} - \bar{a}^{n+\frac12}_{i-1}) = 0$ $\therefore$

$\Rightarrow$ projected back then $(a^{n+1}_{i} - a^{n}_{i}) + \mu\,(a^{n}_{i} - a^{n}_{i-1}) = 0$ $\therefore$ (equivalent)

(2) Let $\mu = a\Delta t/\Delta x$, $\nu = b\Delta t/\Delta y$ then

Define $$\bar{a}^{n}_{i+\frac12,j+\frac12} = \int_{x_i}^{x_{i+1}}\int_{y_j}^{y_{j+1}} a(t,x,y)\,dx\,dy \cdot \frac{1}{\Delta x\Delta y}$$

then,
$$\frac{\partial a}{\partial t} + a\frac{\partial a}{\partial x} + b\frac{\partial a}{\partial y} = 0 \quad \times \int dx\,dy\,dt$$

$$\Rightarrow \Delta x\Delta y\cdot(\bar{a}^{n+1}_{i+\frac12,j+\frac12} - \bar{a}^{n}_{i+\frac12,j+\frac12}) + a(\bar{a}^{n+\frac12}_{i+1,j+\frac12} - \bar{a}^{n+\frac12}_{i,j+\frac12})\Delta y\Delta t$$
$$+ b\,\Delta x\Delta t\,(\bar{a}^{n+\frac12}_{i+\frac12,j+1} - \bar{a}^{n+\frac12}_{i+\frac12,j}) = 0$$

$$\Rightarrow \frac{1}{\Delta t}(\bar{a}^{n+1}_{i+\frac12,j+\frac12} - \bar{a}^{n}_{i+\frac12,j+\frac12}) + a\cdot\frac{1}{\Delta x}\underbrace{(\bar{a}^{n+\frac12}_{i+1,j+\frac12} - \bar{a}^{n+\frac12}_{i,j+\frac12})}_{①}$$
$$+ b\cdot\frac{1}{\Delta y}\underbrace{(\bar{a}^{n+\frac12}_{i+\frac12,j+1} - \bar{a}^{n+\frac12}_{i+\frac12,j})}_{②} = 0$$

$$\Rightarrow \bar{a}^{n+1}_{i+\frac12,j+\frac12} = \bar{a}^{n}_{i+\frac12,j+\frac12} - \mu\cdot① - \nu\cdot②$$

In our problem, $i, j \to i-1, j-1$ thus
$$\bar{a}^{n}_{i-\frac12,j-\frac12} = \bar{a}^{n}_{i-\frac12,j-\frac12} - \mu\cdot(\bar{a}^{n+\frac12}_{i,j-\frac12} - \bar{a}^{n+\frac12}_{i-1,j-\frac12}) - \nu\cdot(\bar{a}^{n+\frac12}_{i-\frac12,j} - \bar{a}^{n+\frac12}_{i-\frac12,j-1})$$

By projecting it back,

$$a^{n+1}_{i,j} = a^{n}_{i,j} - \mu\,(a^{n}_{i,j} - a^{n}_{i-1,j}) - \nu\,(a^{n}_{i,j} - a^{n}_{i,j-1})$$

$$a^{n+1}_{i,j} = (1-\mu-\nu)\,a^{n}_{i,j} + \mu\,a^{n}_{i-1,j} + \nu\,a^{n}_{i,j-1}$$

(a) $$u_{i,j}^{n+1} = u_{i,j}^{n} + \frac{\partial u}{\partial t}\cdot\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial t^2}\Delta t^2$$

$$u_{i-1,j}^{n} = u_{i,j}^{n} - \frac{\partial u}{\partial x}\cdot\Delta x + \frac{1}{2}\Delta x^2\frac{\partial^2 u}{\partial x^2} + \cdots$$

$$u_{i,j-1}^{n} = u_{i,j}^{n} - \frac{\partial u}{\partial y}\Delta y + \frac{1}{2}\Delta y^2\frac{\partial^2 u}{\partial y^2} + \cdots$$

$$\Rightarrow \frac{\partial u}{\partial t}\Delta t + \frac{1}{2}\Delta t^2\frac{\partial^2 u}{\partial t^2} + \cancel{O(\Delta t^3)} = -\mu\Delta x\frac{\partial u}{\partial x} - \nu\Delta y\frac{\partial u}{\partial y} + \frac{1}{2}\mu\Delta x^2\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}\nu\Delta y^2\frac{\partial^2 u}{\partial y^2} + \cancel{O(\Delta x^3)} + \cancel{O(\Delta y^3)}$$

$$\Rightarrow \frac{\partial u}{\partial t} + \mu\frac{\Delta x}{\Delta t}\frac{\partial u}{\partial x} + \nu\frac{\Delta y}{\Delta t}\frac{\partial u}{\partial y} = \frac{1}{2}\mu\frac{\Delta x^2}{\Delta t}\cdot\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}\nu\frac{\Delta y^2}{\Delta t}\frac{\partial^2 u}{\partial y^2} - \frac{1}{2}\Delta t\frac{\partial^2 u}{\partial t^2}$$

$$* \quad \frac{\partial^2 u}{\partial t^2} = a^2\frac{\partial^2 u}{\partial x^2} + b^2\frac{\partial^2 u}{\partial y^2} + 2ab\frac{\partial^2 u}{\partial x\partial y}$$

Finally,

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = \frac{1}{2}(a\Delta x - a^2\Delta t)\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}(b\Delta y - b^2\Delta t)\frac{\partial^2 u}{\partial y^2} - ab\Delta t\frac{\partial^2 u}{\partial x\partial y}$$

or

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} = \frac{1}{2}a\Delta x(1-\mu)\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}b\Delta y(1-\nu)\frac{\partial^2 u}{\partial y^2} - ab\Delta t\frac{\partial^2 u}{\partial x\partial y}$$

The modified equation has additional diffusion terms which are proportional to Δx, Δy, and Δt with respectively.