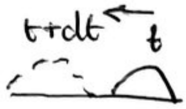
Numerical Exercises 1 2024

1) $$u_t \underbrace{- a(t) u_x}_{\text{advective term}} \underbrace{- \varepsilon u_{xx}}_{\text{diffusive term}} = 0$$

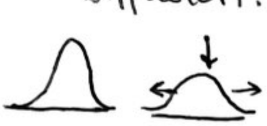
Linear: each variable is raised to the power of one

~~Advection: the flow of a fluid and of particles downstream / alongside the bulk flow~~

Advection: the bulk movement of a fluid ~~or~~ or energy / other physical quantities. Notably, its the movement of the entire envelope / wave.



Diffusion: the net movement of a physical quantity (eg energy) or particles from a region of high concentration to a region of lower concentration. It arises from statistical mechanics and causes the wave to spread out.



This equation is called the linear advection diffusion equation as it evaluates how the velocity of a fluid evolves in time when both diffusion and advection are present.

2)

(2.80) $$\delta_t U_j^{n+1/2} = U_j^{n+1} - U_j^n$$

$$= \left[u + \cancel{\tfrac{1}{2}\Delta t\, u_t} + \tfrac{1}{2}\left(\tfrac{1}{2}\Delta t\right)^2 u_{tt} + \cancel{\tfrac{1}{6}\left(\tfrac{1}{2}\Delta t\right)^3} u_{ttt} + \dots \right]_j^{n+1/2}$$

$$- \left[\cancel{u} - \cancel{\tfrac{1}{2}\Delta t\, u_t} + \tfrac{1}{2}\left(-\tfrac{1}{2}\Delta t\right)^2 u_{tt} + -\cancel{\tfrac{1}{6}\left(\tfrac{1}{2}\Delta t\right)^3} u_{ttt} + \dots \right]_j^{n+1/2}$$

$$=$$

2)

(2.80)

$$\delta_t u_j^{n+1/2} = U_j^{n+1} - U_j^n$$

$$= \left[\cancel{u} + \tfrac{1}{2}\Delta t\, u_t + \cancel{\tfrac{1}{2}(\tfrac{1}{2}\Delta t)^2 u_{tt}} + \tfrac{1}{6}(\tfrac{1}{2}\Delta t)^3 u_{ttt} + \dots\right]_j^{n+1/2}$$

even terms cancel

$$- \left[\cancel{u} - \tfrac{1}{2}\Delta t\, u_t + \cancel{\tfrac{1}{2}(\tfrac{1}{2}\Delta t)^2 u_{tt}} - \tfrac{1}{6}(\tfrac{1}{2}\Delta t)^3 u_{ttt} + \dots\right]_j^{n+1/2}$$

$$= \left[2(\tfrac{1}{2}\Delta t\, u_t) + 2(\tfrac{1}{6}(\tfrac{1}{2}\Delta t)^3 u_{ttt}) + \dots\right]_j^{n+1/2}$$

$$= \left[\Delta t\, u_t + \tfrac{1}{24}(\Delta t)^3 u_{ttt} + \dots\right]_j^{n+1/2}$$

(2.81)

$\boxed{\text{NB: } u_{4x} = u_{xxxx}}$

$$\delta_x^2 u_j^{n+1} = \Delta_{+x} u(x,t) - \Delta_{-x} u(x,t)$$

① $$\Delta_{+x} u(x,t) = u(x+\Delta x, t) - u(x,t)$$

$$= \cancel{u} + \Delta x\, u_x + \tfrac{1}{2}(\Delta x)^2 u_{xx} + \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \tfrac{1}{24}(\Delta x)^4 u_{4x} + O((\Delta x)^5) - \cancel{u}$$

$$= \Delta x\, u_x + \tfrac{1}{2}(\Delta x)^2 u_{xx} + \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \tfrac{1}{24}(\Delta x)^4 u_{4x} + O((\Delta x)^5)$$

②
$$-\Delta_{-x} u(x,t) = u(x-\Delta x, t) - u(x,t)$$

$$= \cancel{u} - \Delta x\, u_x + \tfrac{1}{2}(\Delta x)^2 u_{xx} - \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \tfrac{1}{24}(\Delta x)^4 u_{4x} + O((\Delta x)^5) - \cancel{u}$$

$$= -\Delta x\, u_x + \tfrac{1}{2}(\Delta x)^2 u_{xx} - \tfrac{1}{6}(\Delta x)^3 u_{xxx} + \tfrac{1}{24}(\Delta x)^4 u_{4x} + O((\Delta x)^5)$$

$$\therefore \delta_x^2 u(x,t) = ① + ②$$

$$= \cancel{\Delta x u_x} + \tfrac{1}{2}(\Delta x)^2 u_{xx} + \cancel{\tfrac{1}{6}(\Delta x)^3 u_{xxx}} + \tfrac{1}{24}(\Delta x)^4 u_{4x}$$
$$\cancel{-\Delta x u_x} + \tfrac{1}{2}(\Delta x)^2 u_{xx} + \cancel{-\tfrac{1}{6}(\Delta x)^3 u_{xxx}} + \tfrac{1}{24}(\Delta x)^4 u_{4x}$$
$$+ O((\Delta x)^5)$$

$$= (\Delta x)^2 u_{xx} + \frac{1}{12}(\Delta x)^4 u_{4x} + O((\Delta x)^5)$$ ← only even terms remain

$$\cancel{\therefore \delta_x^2 u_j^{n+1} = [(\Delta x)^2 u_{xx} + \tfrac{1}{12}}$$

for arbitrary even index n: term $= \dfrac{2}{n!}(\Delta x)^n u_{nx}$

$\therefore$ 6th term $= \dfrac{2}{6!}(\Delta x)^6 u_{6x}$

$$\therefore \delta_{x}\cancel{^2 u(x,t}$$

$$\therefore \delta_x^2 u_j^{n+1} = \left[(\Delta x)^2 u_{xx} + \frac{1}{12}(\Delta x)^4 u_{4x} + \frac{2}{6!}(\Delta x)^6 u_{6x} + \dots\right]_j^{n+1}$$

(2.82)

$$\delta_x^2 u_j^{n+1} = \delta_x^2 u_j^n + \left(\tfrac{1}{2}\Delta t\right)\delta_x^2 u_j^n + \frac{1}{2!}\left(\tfrac{1}{2}\Delta t\right)^2 \delta_x^2 u_j^n$$

$$= \left[(\Delta x)^2 u_{xx} + \tfrac{1}{12}(\Delta x)^4 u_{4x} + \frac{2}{6!}(\Delta x)^6 u_{6x}\right]$$

$$+ \tfrac{1}{2}\Delta t\left[(\Delta x)^2 u_{xxt} + \frac{1}{12}(\Delta x)^4 u_{xxxxt} + \dots\right]$$

$$+ \frac{1}{2}\left(\tfrac{1}{2}\Delta t\right)^2\left[(\Delta x)^2 u_{xxtt} + \dots\right]$$

$$= \frac{2}{6!}(\Delta x)^6 u_{xxxxxx} + \frac{\Delta t(\Delta x)^4}{24} u_{xxxxt} + \frac{(\Delta x)^2}{24}\left[2u_{4x}\cdot(\Delta x)^2 + 3u_{xxtt}(\Delta t)^2\right]$$

$$+ \frac{\Delta t(\Delta x)^2}{2} u_{xxt} + (\Delta x)^2 u_{xx}$$

(4)

$$\theta \delta_x^2 U_j^{n+1} = \theta \overbrace{\left[(\Delta x)^2 u_{xx} + \frac{1}{12} (\Delta x)^4 u_{4x} + \frac{2}{6!} (\Delta x)^6 u_{6x} \right]}^{A}$$

$$+ \frac{1}{2} \Delta t \overbrace{\left[(\Delta x)^2 u_{xxt} + \frac{1}{12} (\Delta x)^4 u_{xxxxt} + \ldots \right]}^{B}$$

$$+ \frac{1}{2} \left(\tfrac{1}{2} \Delta t \right)^2 \overbrace{\left[(\Delta x)^2 u_{xxtt} + \ldots \right]}^{C}$$

$$= \theta A + \frac{1}{2} \Delta t B \theta + \frac{1}{2} \left(\tfrac{1}{2} \Delta t \right)^2 C \theta$$

$$\delta_x^2 u_j^n = A - \tfrac{1}{2} \Delta t B + \frac{1}{2} \left(\tfrac{1}{2} \Delta t \right)^2 C$$

$$\therefore \theta \delta_x^2 u_j^{n+1} + \delta_x^2 u_j^n - \theta \delta_x^2 u_j^n = \theta \left[\cancel{A} + \tfrac{1}{2} \Delta t B + \cancel{\tfrac{1}{2} (\tfrac{1}{2} \Delta t)^2 C} \right]$$

$$+ \left[A - \tfrac{1}{2} \Delta t B + \tfrac{1}{2} (\Delta t)^2 C \right]$$

$$- \theta \left[\cancel{A} - \tfrac{1}{2} \Delta t B + \cancel{\tfrac{1}{2} (\tfrac{1}{2} \Delta t)^2 C} \right]$$

$$= A - \tfrac{1}{2} \Delta t B + \frac{1}{8} (\Delta t)^2 C + \theta \Delta t B$$

$$\boxed{\text{Notation: } u_{4x} = u_{xxxx}}$$

$$= A + \left(\theta - \tfrac{1}{2} \right) \Delta t B + \tfrac{1}{8} (\Delta t)^2 C$$

$$= \left[(\Delta x)^2 u_{xx} + \tfrac{1}{12} (\Delta x)^4 u_{4x} + \frac{2}{6!} (\Delta x)^6 u_{6x} + \ldots \right]$$

$$+ \left(\theta - \tfrac{1}{2} \right) \Delta t \left[(\Delta x)^2 u_{xxt} + \tfrac{1}{12} (\Delta x)^4 u_{xxxxt} + \ldots \right]$$

$$+ \frac{1}{8} (\Delta t)^2 \left[(\Delta x)^2 u_{xxtt} + \ldots \right]$$

(2.83) $T\cancel{(x,t) = \Delta_{+t} u(x,t)} - \delta_x^2 u(x,t)$ (5)

$$T(x,t) = \frac{\Delta_{+t} u(x,t)}{\Delta t} - \frac{\delta_x^2 u(x,t)}{(\Delta x)^2} \quad \text{for the explicit scheme}$$

our scheme: $U_j^{n+1} - U_j^n = \mu\left[\theta \delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n\right]$

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{\left[\theta \delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n\right]}{(\Delta x)^2}$$

from earlier: $U_j^{n+1} - U_j^n = \delta_t u_j^{n+1/2}$

$$\therefore \frac{\delta_t u_j^{n+1/2}}{\Delta t} = \frac{\left[\theta \delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n\right]}{(\Delta x)^2}$$

$\therefore$ the truncation error is : $T_j^{n+1/2} = \dfrac{\delta_t u_j^{n+1/2}}{\Delta t} - \dfrac{\theta \delta_x^2 u_j^{n+1} - (1-\theta)\delta_x^2 u_j^n}{(\Delta x)^2}$

(2.84)

$$T_j^{n+1/2} = \overbrace{\frac{\delta_t u_j^{n+1/2}}{\Delta t}}^{\Phi} - \overbrace{\frac{\theta \delta_x^2 u_j^{n+1} - (1-\theta)\delta_x^2 u_j^n}{(\Delta x)^2}}^{\Psi}$$

$$= \Phi - \Psi$$

$$\Phi = \frac{\cancel{\Delta t}\left[\Delta t\, u_t + \tfrac{1}{24}(\Delta t)^3 u_{ttt} + \ldots\right]_j^{n+1/2}}{\Delta t}$$

$$= u_t + \tfrac{1}{24}(\Delta t)^2 u_{ttt}$$

$$\Psi = \frac{\theta \delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n}{(\Delta x)^2} \qquad \boxed{u_{4x} = u_{xxxx}}$$

$$= \left[u_{xx} + \tfrac{1}{12}(\Delta x)^2 u_{4x} + \tfrac{2}{6!}(\Delta x)^4 u_{6x} + \cdots\right]$$
$$+ (\theta - \tfrac{1}{2})\Delta t \left[u_{xxt} + \tfrac{1}{12}(\Delta x)^{\cancel{4}\,2} u_{xxxxt} + \cdots\right]$$
$$+ \tfrac{1}{8}(\Delta t)^2 \left[u_{xxtt} + \cdots\right]$$

$$\therefore T_j^{n+1/2} = \left[u_t + \tfrac{1}{24}(\Delta t)^2 u_{ttt}\right] - \left[u_{xx} + \tfrac{1}{2}(\Delta x)^2 u_{4x} + \tfrac{2}{6!}(\Delta x)^4 u_{6x}\right]$$
$$\cancel{-(\theta - \tfrac{1}{2})\Delta t\,[u_{xxt} + \tfrac{1}{12}}$$
$$+ (\tfrac{1}{2} - \theta)\Delta t \left[u_{xxt} + \tfrac{1}{12}(\Delta x)^2 u_{xxxxt} + \cdots\right]$$
$$- \tfrac{1}{8}(\Delta t)^2 \left[u_{xxtt} + \cdots\right]$$

$$= \left[u_t - u_{xx}\right] + \left[(\tfrac{1}{2} - \theta)\Delta t\, u_{xxt} - \tfrac{1}{12}(\Delta x)^2 u_{4x}\right]$$
$$+ \left[\tfrac{1}{24}(\Delta t)^2 u_{ttt} - \tfrac{1}{8}(\Delta t)^2 u_{xxtt}\right]$$
$$+ \left[\tfrac{1}{12}(\tfrac{1}{2} - \theta)\Delta t (\Delta x)^2 u_{xxxxt} - \tfrac{2}{6!}(\Delta x)^4 u_{6x}\right] \quad (2.84)$$

3) θ method discretisation

Explicit scheme: ① $\dfrac{U_j^{n+1}-U_j^n}{\Delta t} = \overbrace{\dfrac{\varepsilon\,\delta_x^2 U_j^n}{(\Delta x)^2}}^{\varepsilon u_{xx}} + \overbrace{\dfrac{a^n\left[U_{j+1}^n - U_j^n\right]}{\Delta x}}^{a(t)u_x}$

$\boxed{\begin{array}{l}\text{NB:}\\ a^n = a(t)\\ a^{n+1} = a(t+\Delta t)\end{array}}$

Implicit scheme: ② $\dfrac{U_j^{n+1}-U_j^n}{\Delta t} = \dfrac{\varepsilon\,\delta_x^2 U_j^{n+1}}{(\Delta x)^2} + a^{n+1}\dfrac{\left[U_{j+1}^{n+1} - U_j^{n+1}\right]}{\Delta x}$

θ scheme: $\dfrac{U_j^{n+1}-U_j^n}{\Delta t} = (1-\theta)\,①\, + \theta\,②$

$\therefore$ ~~$U_j^{n+1} - U_j^n$~~

$$U_j^{n+1} - U_j^n = \mu\varepsilon\left[\theta\delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n\right] + \mu\theta a^{n+1}\Delta x\left[U_{j+1}^{n+1} - U_j^{n+1}\right] + \mu(1-\theta)\Delta x\, a^n\left[U_{j+1}^n - U_j^n\right]$$

$\delta_x^2 U_j^n = U_{j+1}^n - 2U_j^n + U_{j-1}^n$ SUB IN

$$U_j^{n+1} - U_j^n = \mu\varepsilon\left[\theta\left(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}\right) + (1-\theta)\delta_x^2 U_j^n\right] + \mu\theta a^{n+1}\Delta x\left[U_{j+1}^{n+1} - U_j^{n+1}\right] + \mu(1-\theta)\Delta x\, a^n\left[U_{j+1}^n - U_j^n\right]$$

$$\left[1 + 2\mu\varepsilon\theta + \mu\theta a^{n+1}\Delta x\right]U_j^{n+1} - \left[\mu\varepsilon\theta + \mu\theta a^{n+1}\Delta x\right]U_{j+1}^{n+1} - U_{j-1}^{n+1}\left[\mu\varepsilon\theta\right]$$
$$= \left[1 + \mu\varepsilon(1-\theta)\delta_x^2 - \mu(1-\theta)\Delta x\, a^n\right]U_j^n$$

~~Using the Thomas algorithm, we can define~~ :

3 continued)

Thomas algorithm: $-a_j U_{j-1} + b_j U_j - c_j U_{j+1} = d_j$

by comparison:
$$-a_j = -\mu\varepsilon\theta$$
$$a_j = \mu\varepsilon\theta$$

$$b_j = 1 + \cancel{2}\,\mu\theta\,[2\varepsilon + a^{n+1}\Delta x]$$

$$c_j = \mu\theta\,[\varepsilon + a^{n+1}\Delta x]$$

$$d_j = 1 + \mu\varepsilon(1-\theta)\,\delta_x^2 U_j^n - \mu(1-\theta)\Delta x\, a^n U_j^n + \mu(1-\theta)\Delta x\, a^n U_{j+1}^n$$

$$\therefore d_j = U_j^n + \mu(1-\theta)\left[\varepsilon\,\delta_x^2 U_j^n + \Delta x\,\Delta_{+x}\, a^n U_j^n\right]$$

ie we have:

$$\cancel{\begin{bmatrix} U_{j-1}^{n+1} \\ U_{j+1}^{n+1} \\ U \end{bmatrix}} \quad \begin{bmatrix} \vdots \\ -a_j U_{j-1}^{n+1} \\ +b_j U_j^{n+1} \\ -c_j U_{j+1}^{n} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \mu(1-\theta)[\varepsilon U_{j-1}^n] \\ U_j^n + \mu(1-\theta)[-2\varepsilon U_j^n - \Delta x\, a^n U_j^n] \\ \mu(1-\theta)[\varepsilon U_{j+1}^n + \Delta x\, a^n U_{j+1}^n] \\ \vdots \end{bmatrix}$$

to solve: define $e_j = \dfrac{c_j}{b_j - a_j e_{j-1}}$ and $f_j = \dfrac{d_j + a_j f_{j-1}}{b_j - a_j e_{j-1}}$

such that: $\boxed{\text{FINAL FORMULATION}}$

after some algebraic rearranging $U_j - e_j U_{j+1} = f_j$

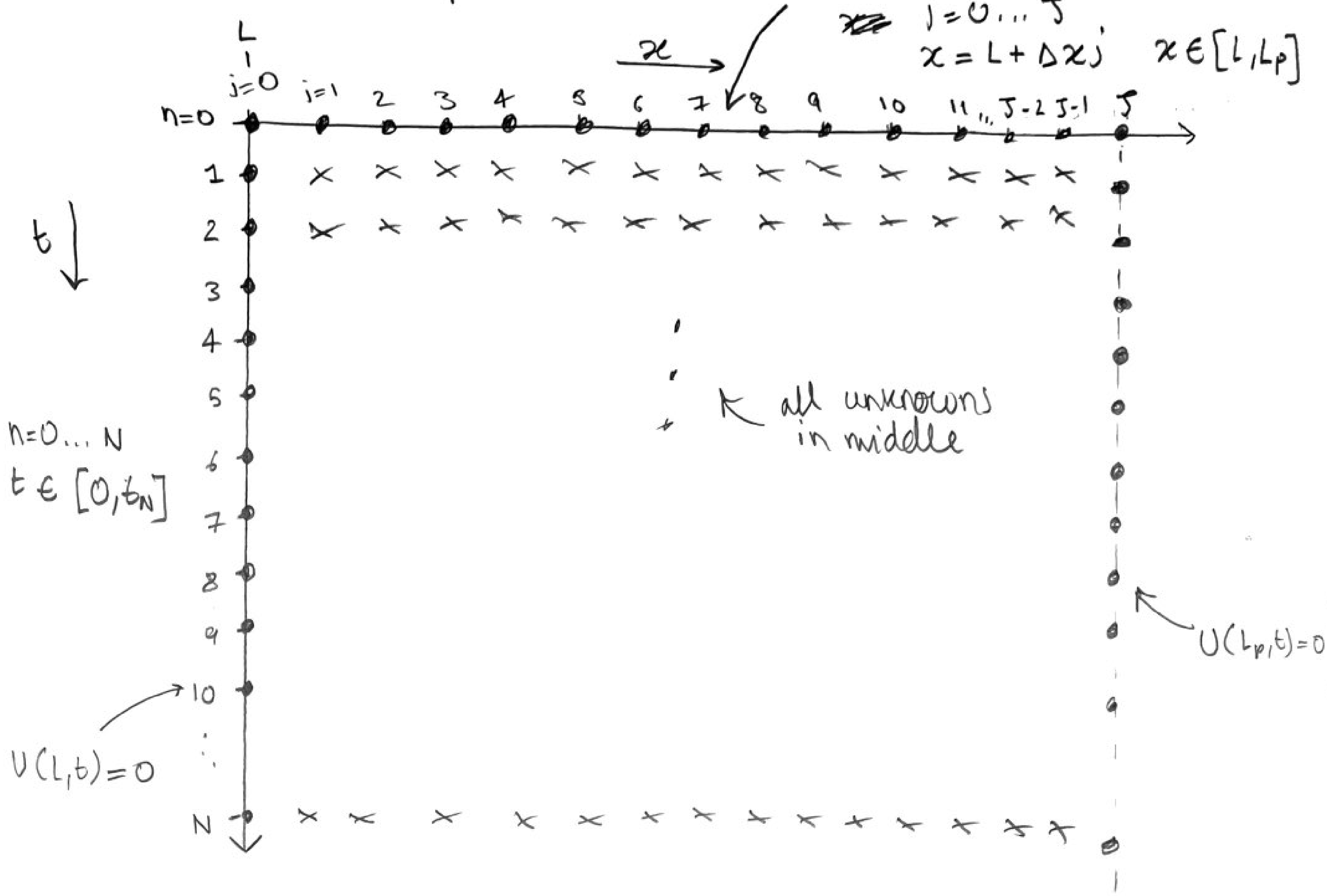
$\boxed{\beta = \mu\theta}$

$$\therefore e_j = \frac{\beta[\varepsilon + a^{n+1}\Delta x]}{1 + \beta[2\varepsilon - \varepsilon e_{j-1} + a^{n+1}\Delta x]}$$

$$f_j = \frac{U_j^n + \mu(1-\theta)\left[\varepsilon(U_{j+1}^n - 2U_j^n + U_{j-1}^n) + \Delta x\, a^n[U_{j+1}^n - U_j^n]\right] + \mu\varepsilon\theta f_{j-1}}{1 + \mu\theta(2\varepsilon + a^{n+1}\Delta x - \varepsilon e_{j-1})}$$

3) continued)

The spacetime mesh $u(x,0) = u_0(x)$



● = knowns
× = unknowns

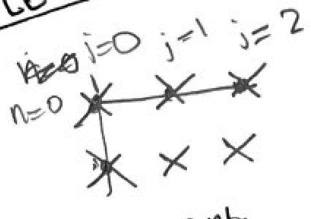
Near the boundary: set $U(L,t) = U(L_p, t) = 0$ for all times t

$u(x,0) = u_0(x)$ ~~no point in doing this as it is already known~~

we only want to iterate from $t = 0 \dots N$ and $j = 1 \dots J-1$

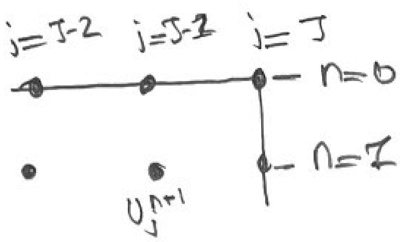
such that $U(j-1)$ or $U(j+1)$ is on the boundary and not outside it.

TOP LEFT



- the six point stencil for $n=0, j=1$
- cannot do $n=0, j=0$ as $U(j-1)$ would make $j=-1$ which is outside the boundary

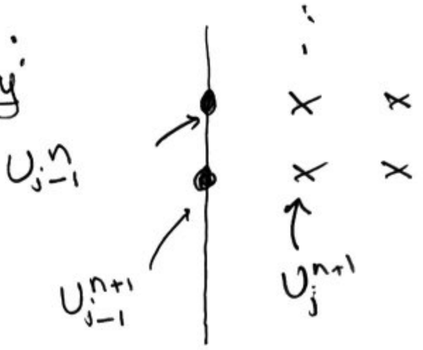
TOP RIGHT



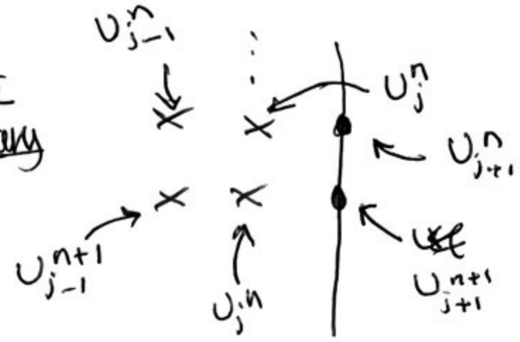
Six point stencil for $n=0$, $j = J-1$

left boundary:

$j = 1$
$n = n$



right boundary



$j = J-1$
$n = \cancel{2}\, n$ ~~where~~

4)

Relevant code: explicit_scheme_figure_2.2.py

The figures generated by the code ~~at the~~ are shown overleaf.

~~Stability properties of the explicit scheme~~

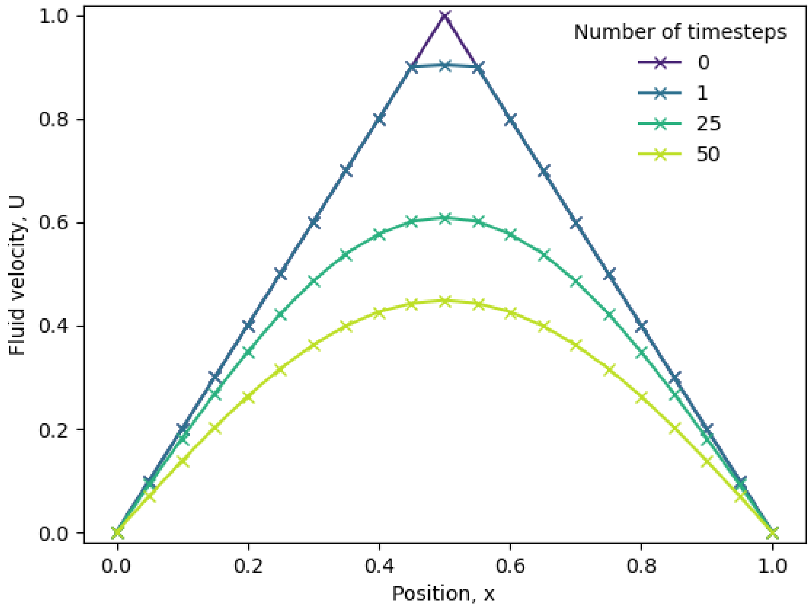


Figure 1: Stable Explicit scheme for J=20, dt=0.0012 and dx=0.05. μ=0.48 so the solution is just in the stable regime of $\mu \leq 0.5$.

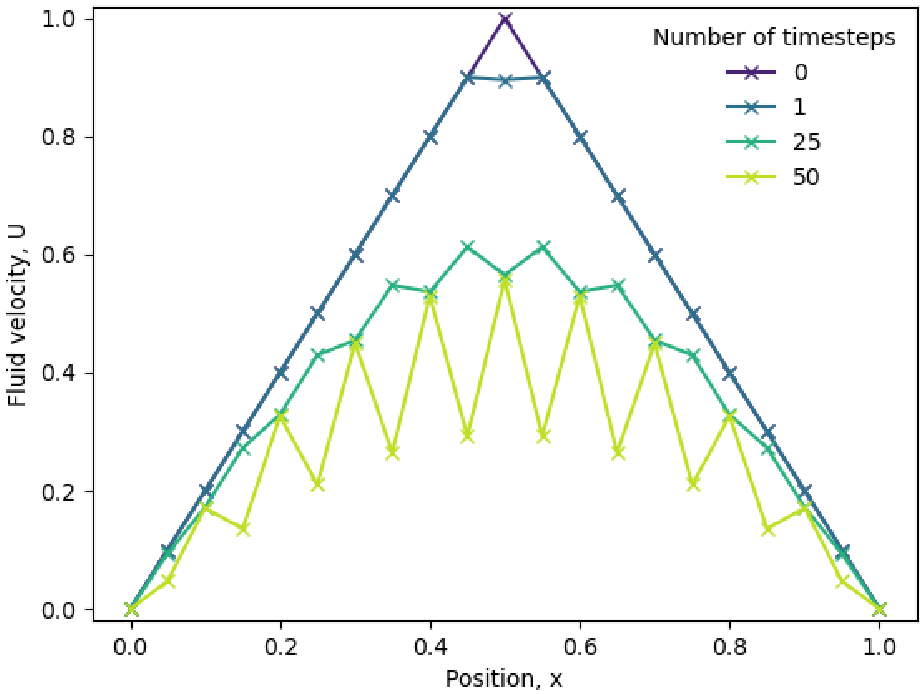


Figure 2: The unstable explicit scheme for J=20, dt=0.0013 and dx=0.05. μ=0.52 so the solution is past the stability threshold of μ=0.5 and the simulation fails to converge upon the solution.

4 continued)

Stability properties of the explicit scheme

$$U_j^n = \lambda^n \exp(ikj\Delta x)$$

$$\downarrow$$

$$\lambda = 1 - 4\mu \sin^2\left(\tfrac{1}{2}k\Delta x\right)$$

~~if $|\lambda \geq 1|$:~~

if $|\lambda \geq 1|$: λ^n grows with each timestep causing the error to increase as a function of time. This makes the code fundamentally unstable.

if $|\lambda \leq 1|$: λ^n decays with time and ~~it is~~ the regime is stable

$\therefore$ the stability criterion is: $|1 - 4\mu| \leq 1$

$\hookrightarrow \mu \leq 1/2$ $\qquad \mu = \dfrac{\Delta t}{\Delta x^2}$ SUB IN

$\therefore \quad \Delta t \leq 1/2(\Delta x)^2$

The explicit scheme is only stable when $\Delta t \leq 1/2(\Delta x)^2$

$\therefore$ if you increase the resolution of the spatial grid, you need to greatly reduce the timestep in order to fulfill this condition.

$\hookrightarrow$ increasing the resolution of the scheme is computationally costly.

Explicit scheme of (1)

$$u_t - a(t)u_t - \varepsilon u_{xx} = 0$$

$\downarrow$ SUB IN equations

$$\boxed{\begin{aligned} u_t &\approx \frac{U_j^{n+1} - U_j^n}{\Delta t} \\ u_x &\approx \frac{U_{j+1}^n - U_j^n}{\Delta x} \\ u_{xx} &\approx \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{(\Delta x)^2} \end{aligned}}$$

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{a(t)\left[U_{j+1}^n - U_j^n\right]}{\Delta x} + \frac{\varepsilon\left[U_{j+1}^n - 2U_j^n + U_{j-1}^n\right]}{\Delta x^2}$$

$\downarrow$ 1) $\times \Delta t$
2) move U_j^n to RHS
3) rearrange

we get: $U_j^{n+1} = U_j^n + \Delta x \mu \, \cancel{a(t)}\, a^n \left[U_{j+1}^n - U_j^n\right] + \varepsilon\mu\left[U_{j+1}^n - 2U_j^n + U_{j-1}^n\right]$ $\quad \boxed{a(t) = a^n}$

5) ~~Code: theta_white.py~~

~~I we have instead used the Thomas algorithm to solve to the system~~

~~Stability properties of θ scheme~~

4 continued) The maximum principle states that the θ scheme converges when $\Delta x, \Delta t \to 0$ provided that:

$$\mu(1-\theta) \leq 1/2$$

$$\mu \leq \frac{1}{2}\left(\frac{1}{1-\theta}\right)$$

within the interval: $U_{min} \leq U_j^n \leq U_{max}$

explicit scheme: $\theta = 0 \Rightarrow \mu \leq 1/2$

~~Combining this with the stability criterion you obtain the following plot~~

$\therefore$ the maximum principle also gives the same result as the Fourier Analysis

5) code: theta_while.py } uses Thomas algorithm to solve the system

<u>stability properties of the θ scheme</u>

$$\boxed{\begin{aligned} a_j &= \mu\varepsilon\theta \\ b_j &= 1+\mu\theta(2\varepsilon + a^{n+1}\Delta x) \\ c_j &= \mu\theta(\varepsilon + a^{n+1}\Delta x) \end{aligned}}$$

$$-a_j U_{j-1}^{n+1} + b_j U_j^{n+1} - c_j U_{j+1}^{n+1} = \mu(1-\theta)[\varepsilon U_{j-1}^n]$$
$$+ [U_j^n + \mu(1-\theta)(-2\varepsilon U_j^n - \Delta x\, a^n U_j^n)]$$
$$+ \mu(1-\theta)[\varepsilon U_{j+1}^n + \Delta x\, a^n U_{j+1}^n]$$

$$U_j^n = \lambda^n \exp(ikj\Delta x)$$

$$U_{j+1}^n = \lambda^n \exp(ik\cancel{j\Delta x + \Delta x}(j+1)\Delta x) \quad \therefore \quad \frac{U_{j+1}^n}{U_j^n} = e^{ik\Delta x}$$

~~dividing RHS~~ similarly: $\dfrac{U_{j-1}^n}{U_j^n} = e^{-ik\Delta x}$, $\dfrac{U_j^{n+1}}{U_j^n} = \lambda$

dividing entire equation by U_j^n

$$-a_j e^{-ik\Delta x}\lambda + \lambda b_j \cancel{e} - c_j e^{ik\Delta x}\lambda = \varepsilon\mu(1-\theta)e^{-ik\Delta x}$$
$$+ (1 + \mu(1-\theta)(-2\varepsilon - \Delta x\, a^n))$$
$$\cancel{+\mu(1-\theta)[\varepsilon U_{j+1}^n + \Delta x a^n]}$$
$$+ \mu(1-\theta)[\varepsilon e^{ik\Delta x} + \Delta x\, a^n e^{ik\Delta x}]$$

<u>Diffusion only:</u>

$a(t) = 0$ for all times t

$$\therefore a_j = \mu\varepsilon\theta \quad b_j = 1 + 2\varepsilon\mu\theta = 1 + 2a_j \quad c_j = \mu\varepsilon\theta = a_j$$

$$-a_j e^{-ik\Delta x}\lambda + \lambda(1+2a_j) - a_j e^{ik\Delta x}\lambda = \varepsilon\mu(1-\theta)e^{-ik\Delta x}$$
$$+ [1 + \mu(1-\theta)(-2\varepsilon)]$$
$$+ \mu(1-\theta)\varepsilon e^{ik\Delta x}$$

$$-a_j\lambda(e^{ik\Delta x} + e^{-ik\Delta x}) + \lambda(1+2a_j) = \varepsilon\mu(1-\theta)[e^{ik\Delta x} + e^{-ik\Delta x}]$$
$$+ 1 - 2\varepsilon\mu(1-\theta)$$

5 continued)

$$\lambda\left[-2\cos(k\Delta x)a_j + 1 + 2a_j\right] = 2\mu\varepsilon(1-\theta)\cos(k\Delta x) + 1 - 2\varepsilon\mu(1-\theta)$$

$$\lambda\left[1+2a_j(1-\cos k\Delta x)\right] = -2\varepsilon\mu(1-\theta)\cancel{\cos}\left[1-\cos(k\Delta x)\right] + 1$$

$$\lambda\left[1+2a_j \cancel{\sin}\cdot 2\sin^2\left(\frac{k\Delta x}{2}\right)\right] = 1-4\mu\varepsilon(1-\theta)\sin^2\left(\frac{k\Delta x}{2}\right)$$

$$\lambda = \frac{1-4\mu\varepsilon(1-\theta)\sin^2\left(\frac{k\Delta x}{2}\right)}{1+4a_j\sin^2\left(\frac{k\Delta x}{2}\right)}$$

$a_j = \mu\varepsilon\theta$

sub in

$$= \frac{1-4\mu\varepsilon(1-\theta)\sin^2\left(\frac{k\Delta x}{2}\right)}{1+4\mu\varepsilon\sin^2\left(\frac{k\Delta x}{2}\right)}$$

λ is unstable when $\lambda \geq 1$ as λ^n blows up. Since λ is a ~~top heavy~~ bottom heavy fraction, $\lambda \leq 1$, so this condition is never met.

to be real: $\lambda > -1$

$\therefore -1 \leq \lambda \leq 1$ ie ~~lambda~~ λ ~~is~~ has to be bounded within this range ~~if we want~~ in order to have ~~a~~ stability

$\underline{\lambda \leq -1}$

$$1-4\mu\varepsilon(1-\theta)\sin^2\left(\frac{k\Delta x}{2}\right) \leq -\left(1+4\theta\mu\varepsilon\sin^2\left(\frac{k\Delta x}{2}\right)\right)$$

$$4\mu\varepsilon(1-2\theta)\sin^2\left(\frac{k\Delta x}{2}\right) \geq 2$$

worst case: $\sin\left(\frac{k\Delta x}{2}\right) = 1$

$$4\mu\varepsilon(1-2\theta) \geq 2$$

$$\mu(1-2\theta) \geq \tfrac{1}{2}\varepsilon \quad \text{] condition for instability}$$

$$\mu \leq \frac{1}{2\varepsilon(1-2\theta)}$$

~~: in the range~~

5) continued) in the range $0 \le \theta \le 1/2$ the scheme is unconditionally stable as $(1-2\theta)$ is always negative and therefore $\mu > \frac{1}{2\varepsilon(1-2\theta)}$

$0 \le \theta \le 1/2$: scheme is conditionally stable if

$$\mu\varepsilon(1-2\theta) < 1/2$$

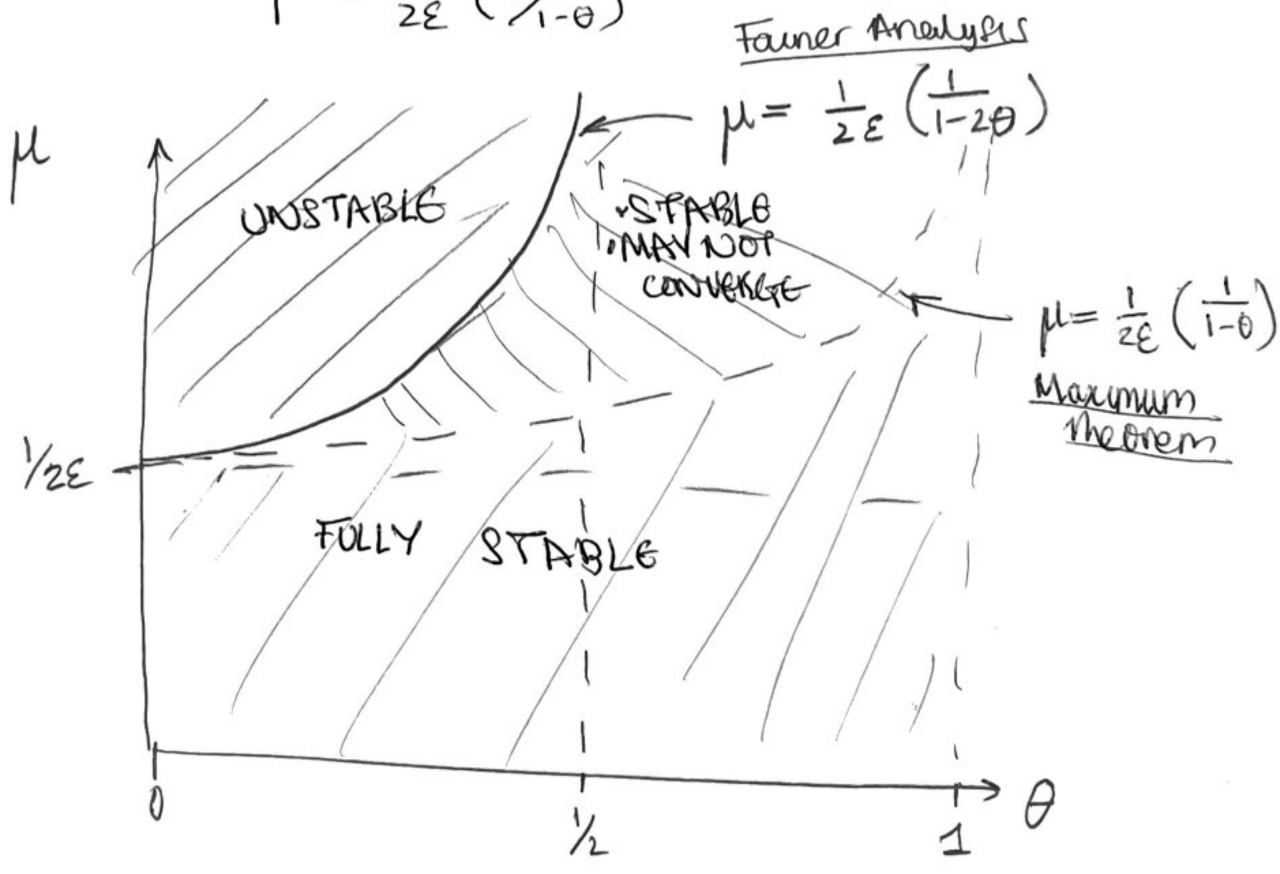
$$\cancel{\mu > \frac{1}{2\varepsilon}\left(\frac{1}{1-2\theta}\right)}$$

$$\mu \le \frac{1}{2\varepsilon}\left(\frac{1}{1-2\theta}\right)$$

Maximum theorem: scheme converges when $\Delta x \Delta t \to 0$ if

$$\mu\varepsilon(1-\theta) \le 1/2$$

$$\mu \le \frac{1}{2\varepsilon}\left(1/_{1-\theta}\right)$$



5 continued)

<u>Advection scheme only</u>

$\varepsilon = 0$

$a_j = 0 \qquad b_j = 1 + a^{n+1}\Delta x \mu\theta \qquad c_j = \mu\theta a^{n+1}\Delta x$

$= 1 + c_j$

~~$(1+c_j)\lambda^{n+1} \exp(ikj$~~

$0 + \cancel{b_j}\lambda(1+c_j) - c_j e^{ik\Delta x}\lambda = 0 + (1 - \mu\Delta x a^n(1-\theta))$
$+ \mu(1-\theta)\left[\Delta x a^n e^{ik\Delta x}\right]$

~~$\lambda + c_j(\lambda$~~

$\lambda\left[1 + c_j - c_j e^{ik\Delta x}\right] = 1 - \mu\Delta x a^n(1-\theta)$
$+ \mu\Delta x a^n(1-\theta)e^{ik\Delta x}$

$\lambda\left[1 + c_j - c_j e^{ik\Delta x}\right] = 1 + \mu\Delta x a^n(1-\theta)\left[e^{ik\Delta x} - 1\right]$

$$\lambda = \frac{1 + \mu\Delta x a^n(1-\theta)\left[e^{ik\Delta x} - 1\right]}{1 + c_j(1 - e^{ik\Delta x})}$$

$c_j = \mu\theta a^{n+1}\Delta x$

~~let $\gamma = \mu\theta\Delta x(1-\theta)$~~

~~$= 1 + \gamma a^n$~~

$$= \frac{1 + \mu\Delta x a^n(1-\theta)\left[e^{ik\Delta x} - 1\right]}{1 + \mu\theta a^{n+1}\Delta x(1 - e^{ik\Delta x})}$$

Note that: when $e^{ik\Delta x} = 1$

$$\lambda = \frac{1 + \cancel{\mu\Delta x a^n(1-\theta)(1-1)}}{1 + \cancel{\mu\theta a^{n+1}\Delta x(1-1)}} = 1$$

ie $\lambda^n = 1^n = 1$ meaning that the amplitude error is zero.

5 continued) ~~let $a^n = a^{n+1} =$ ie a is a constant~~ $a^n = a^{n+1} = a$

ie a is a constant

then $\lambda = \dfrac{1 + \mu\Delta x a(1-\theta)[e^{ik\Delta x} - 1]}{1 + \mu\theta a\Delta x(1 - e^{ik\Delta x})}$

$= \dfrac{1 + \mu\Delta x a(e^{ik\Delta x} - 1)}{1 + \mu\theta a\Delta x(1 - e^{ik\Delta x})}^{=-1} - \dfrac{\theta(e^{ik\Delta x} - 1)}{1 + \mu\theta a\Delta x(1 - e^{ik\Delta x})}$

$= -1 - \dfrac{\theta(e^{ik\Delta x} - 1)}{1 + \mu\theta\Delta x(1 - e^{ik\Delta x})}$

$|\lambda| \le 1$

$\therefore \left| -1 - \dfrac{\theta(e^{ik\Delta x} - 1)}{1 + \mu\theta\Delta x(1 - e^{ik\Delta x})} \right| \le 1$

$a^n = a^{n+1} = a$ ie a is a constant

$\lambda = \dfrac{1 + \mu\Delta x a(1-\theta)[e^{ik\Delta x} - 1]}{1 + \mu\theta a\Delta x(1 - e^{ik\Delta x})}$

$= \dfrac{1 - \theta\mu\Delta x a[e^{ik\Delta x} - 1]}{(1 - \mu\theta a\Delta x(e^{ik\Delta x} - 1))}^{=1} + \dfrac{\mu\Delta x a(e^{ik\Delta x} - 1)}{1 + \mu\theta a\Delta x(1 - e^{ik\Delta x})}$

$= \dfrac{1 + \mu\Delta x a(e^{ik\Delta x} - 1)}{1 + \mu\theta a\Delta x(1 - e^{ikx})}$ let $\sigma = \mu a\Delta x$

$= 1 + \dfrac{1 + \sigma(e^{ik\Delta x} - 1)}{1 + \sigma\theta(1 - e^{ik\Delta x})}$

$= \dfrac{1 - \sigma\theta(e^{ik\Delta x} - 1) + \sigma(e^{ik\Delta x} - 1)}{1 + \sigma\theta(1 - e^{ik\Delta x})}$

$$= \frac{1 + \sigma(1-\theta)\left[e^{ik\Delta x} - 1\right]}{1 + \sigma\theta\left(1 - e^{ik\Delta x}\right)} \qquad \sigma = \mu a \Delta x$$

$|\lambda| \leq 1$

$$\left| \frac{2 + \sigma(1-\theta)\left[e^{ik\Delta x} - 1\right]}{1 + \sigma\theta\left(1 - e^{ik\Delta x}\right)} \right| \leq 1$$

$$\sqrt{\left(\frac{2 + \sigma(1-\theta)\left[e^{-ik\Delta x} - 1\right]}{1 + \sigma\theta\left(1 - e^{-ik\Delta x}\right)} \times \frac{2 + \sigma(1-\theta)\left[e^{ik\Delta x} - 1\right]}{1 + \sigma\theta\left(1 - e^{ik\Delta x}\right)} \right)} \leq 1$$

$|a+b| \leq |a| + |b|$

$|\lambda| \leq \cancel{1}$

$|a| + |b| \leq |a| + |b|$

$$\lambda = 1 + \frac{\mu\Delta x a\left(e^{ik\Delta x} - 1\right)}{1 + \mu\theta a\Delta x\left(1 - e^{ik\Delta x}\right)} \qquad \sigma = \mu a \Delta x$$

$$= 1 + \frac{\sigma\left(e^{ik\Delta x} - 1\right)}{1 + \sigma\theta\left(1 - e^{ik\Delta x}\right)}$$

$|\lambda| \leq 1$

$$\left| 1 + \frac{\sigma\left(e^{ik\Delta x} - 1\right)}{1 + \sigma\theta\left(1 - e^{ik\Delta x}\right)} \right| \leq |1| + \left| \frac{\sigma\left(e^{ik\Delta x} - 1\right)}{1 + \sigma\theta\left(1 - e^{ik\Delta x}\right)} \right|$$

assuming $|a| + |b| \leq 1$

$$1 + \left| \frac{\sigma\left(e^{ik\Delta x} - 1\right)}{1 + \sigma\theta\left(1 - e^{ik\Delta x}\right)} \right| \leq 1$$

then $\left| \dfrac{\sigma(e^{ik\Delta x}-1)}{1+\sigma\theta(1-e^{ik\Delta x})} \right| \leq 0$

$|\sigma(e^{ik\Delta x}-1)| \leq 0$

$\cancel{\sigma 2}\ \sigma\sqrt{(e^{-ik\Delta x}-1)(e^{ik\Delta x}-1)} \leq 0$

$\cancel{\sigma}\sqrt{1-e^{-ik\Delta x}-e^{ik\Delta x}+1} \leq 0$

$\cancel{\sigma}\sqrt{2 - (e^{ik\Delta x}+e^{-ik\Delta x})} \leq 0$

$\sqrt{2-2\cos(k\Delta x)} \leq 0$

$\sqrt{\cancel{2}(1-\cos(k\Delta x))} \leq 0$

$1-\cos k\Delta x \leq 0$??

$\cancel{\cos k\Delta x}$

6) code: theta_while.py using the different initial conditions

$\varepsilon = 1\times10^{-3}$

$f_1(x) = (1-x)^4(1+x)$ and

$f_2(x) = (1-x)^4(1+x)\left(\sum_0^{k=3} b_k\phi_k + c\right)$

I set the coefficients to be equal to that shown within the question. When generating the random coefficients b_k, I set the seed of np.random to be 11 in order to ensure reproducibility. This gave b values of [0.18026969, 0.01947524, 0.46321853, 0.72493393]

The plots ~~from~~ (Figures 3-8) are shown overleaf. and, in order to generate them, I set N=100 (dt = 0.01) and J = 20000 (dx = 0.0001). This gave ~~a~~ $\mu = 1\times10^6$ ie a very high μ value for which the explicit scheme was unfavourable. When $\theta \geq 0.5$, the plots converged correctly upon the expected solution. Reducing θ below this value caused the simulations to quickly enter ~~with~~ an unstable regime, resulting in oscillations being observed within the simulations.

~~I also~~ To create ~~figures~~ Figures 9-12, I set N=100 and J = 175. This gave dx = 0.0114 and dt = 0.01, resulting in a μ value of 76.56. I then ~~varied θ~~ set θ to 0 or 1, highlighting the fact that both simulations yield the same results. This ~~suggests~~ that, in this case, ~~θ is~~ the simulation is stable for all values of θ and verifies that our results yield the same results as the explicit scheme.

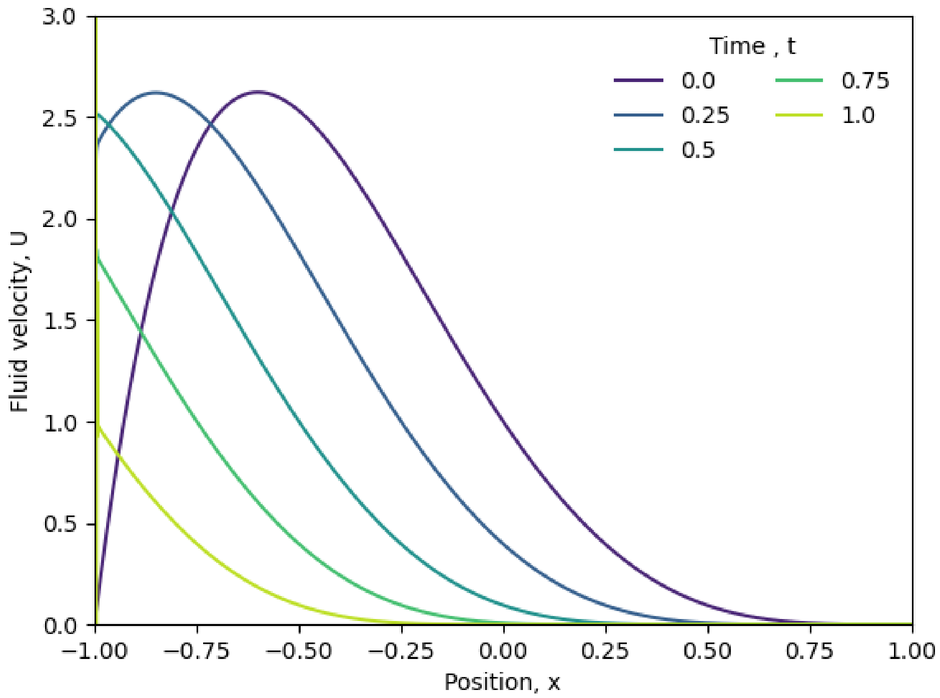


Figure 3: A plot of position vs velocity for ϑ=0.45, μ= 1000000 and $u(x,0) = (1-x)^4(1+x)$

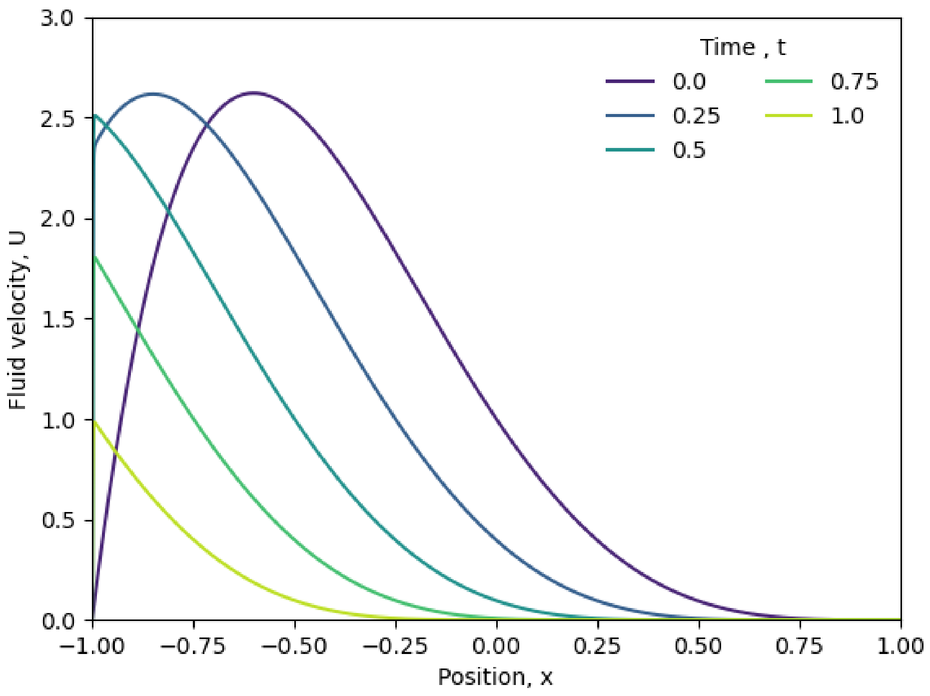


Figure 4: A plot of position vs velocity for ϑ=0.5, μ= 1000000 and $u(x,0) = (1-x)^4(1+x)$

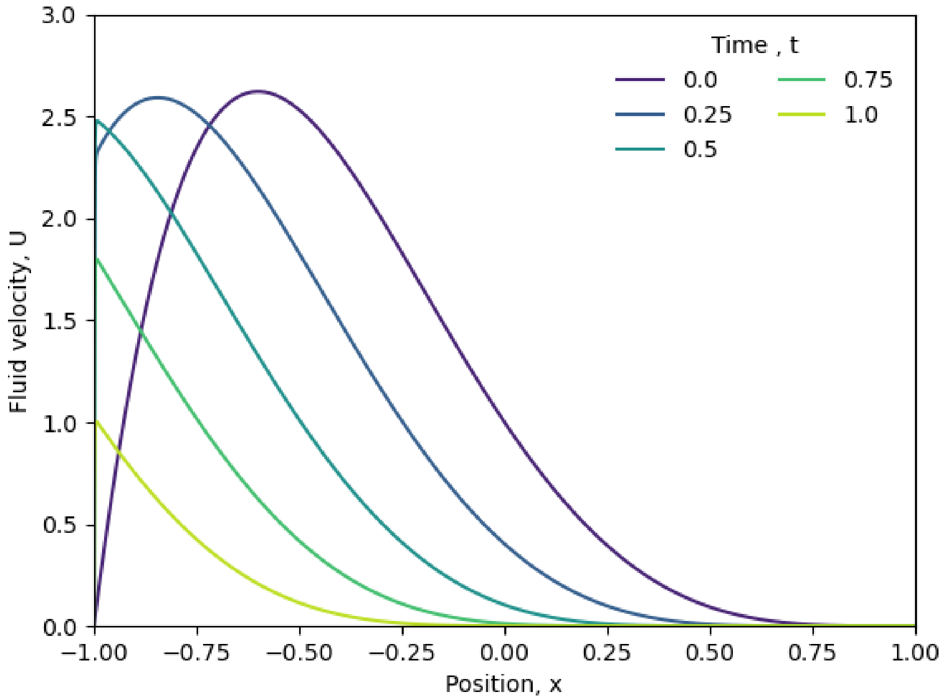


Figure 5: A plot of position vs velocity for ϑ=1.0, μ= 1000000 and $u(x,0) = (1-x)^4(1+x)$

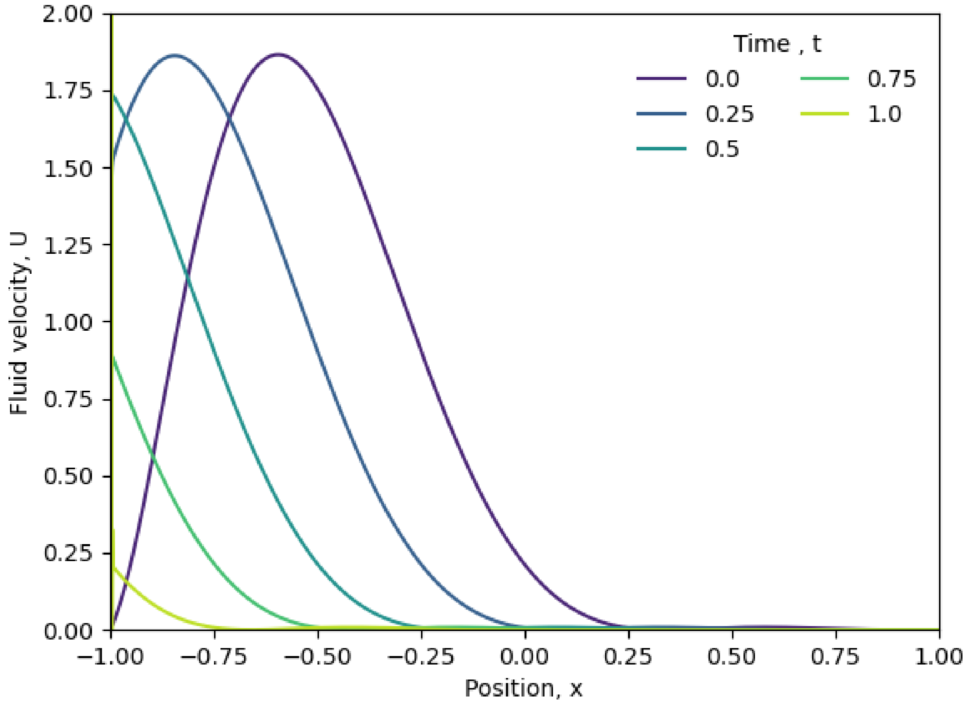


Figure 6: A plot of position vs velocity for ϑ=0.45, μ= 1000000 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k \varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

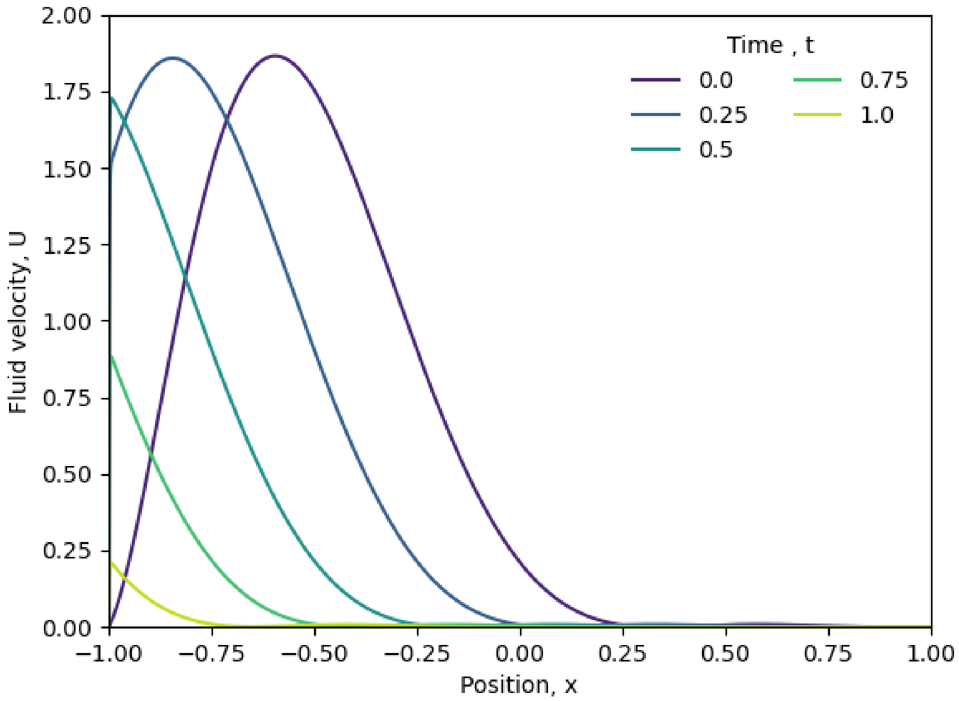


Figure 7: A plot of position vs velocity for ϑ=0.5, μ= 1000000 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

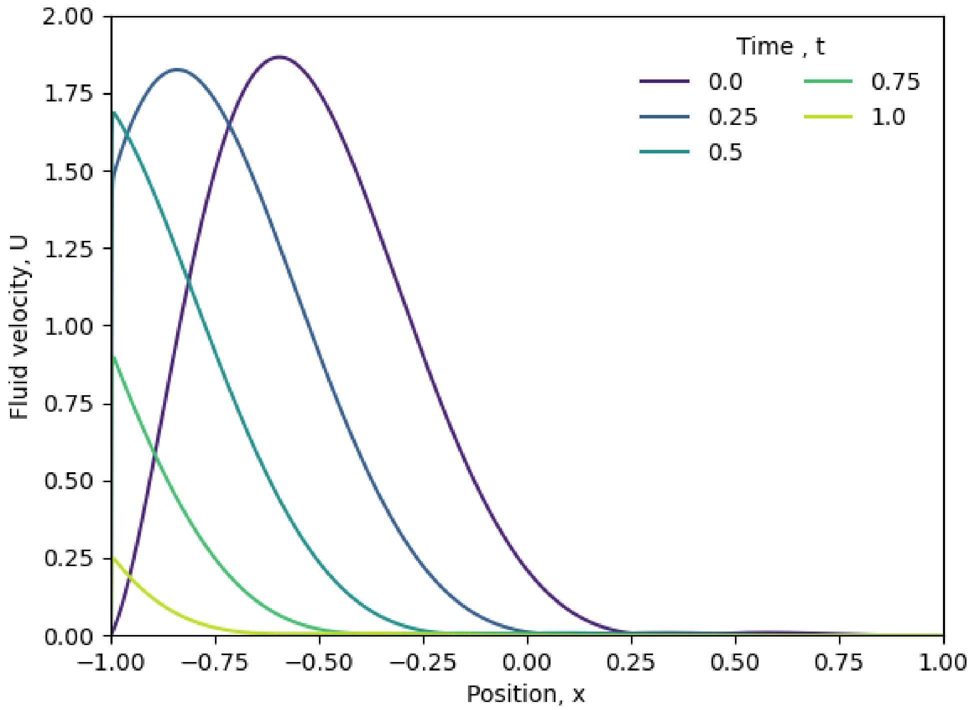


Figure 8: A plot of position vs velocity for ϑ=1.0, μ= 1000000 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

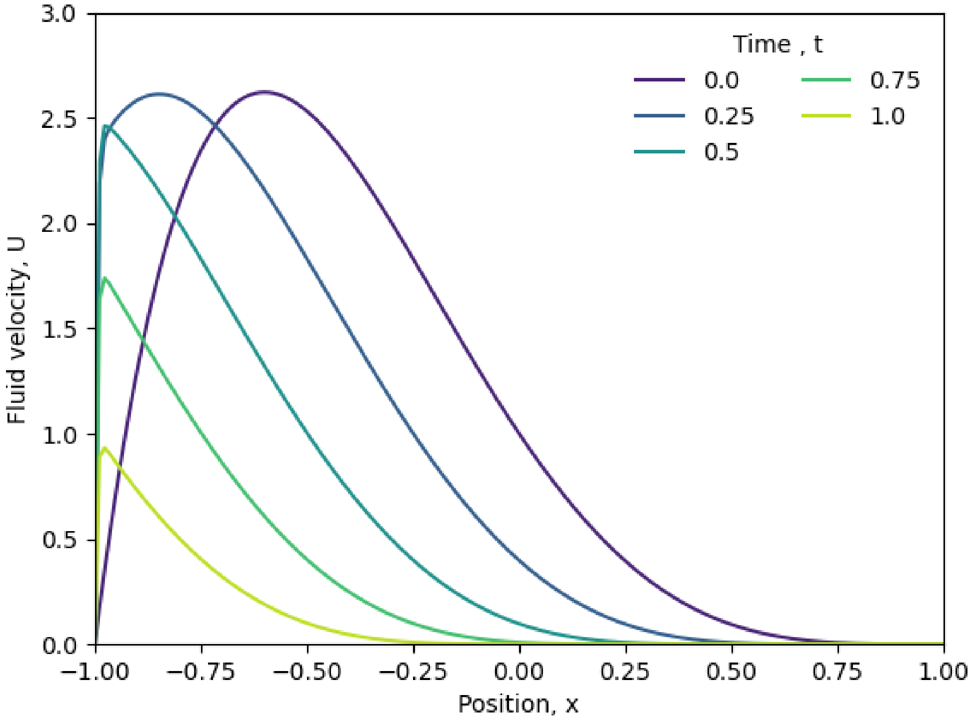


Figure 9: A plot of position vs velocity for ϑ=0.0, μ= 76.56 and $u(x,0) = (1-x)^4(1+x)$

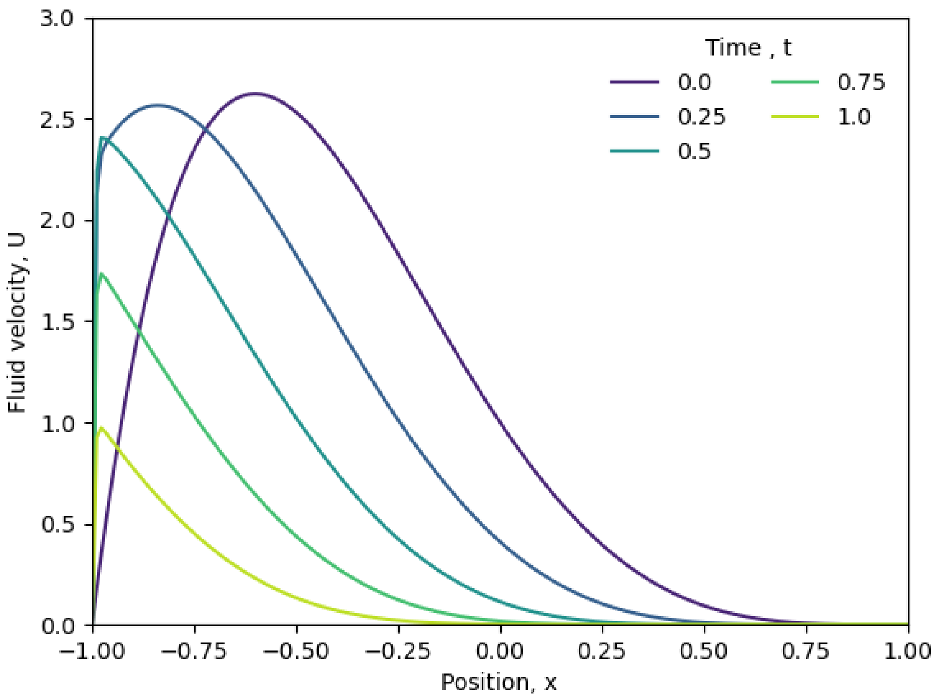


Figure 10: A plot of position vs velocity for ϑ=1.0, μ= 76.56 and $u(x,0) = (1-x)^4(1+x)$

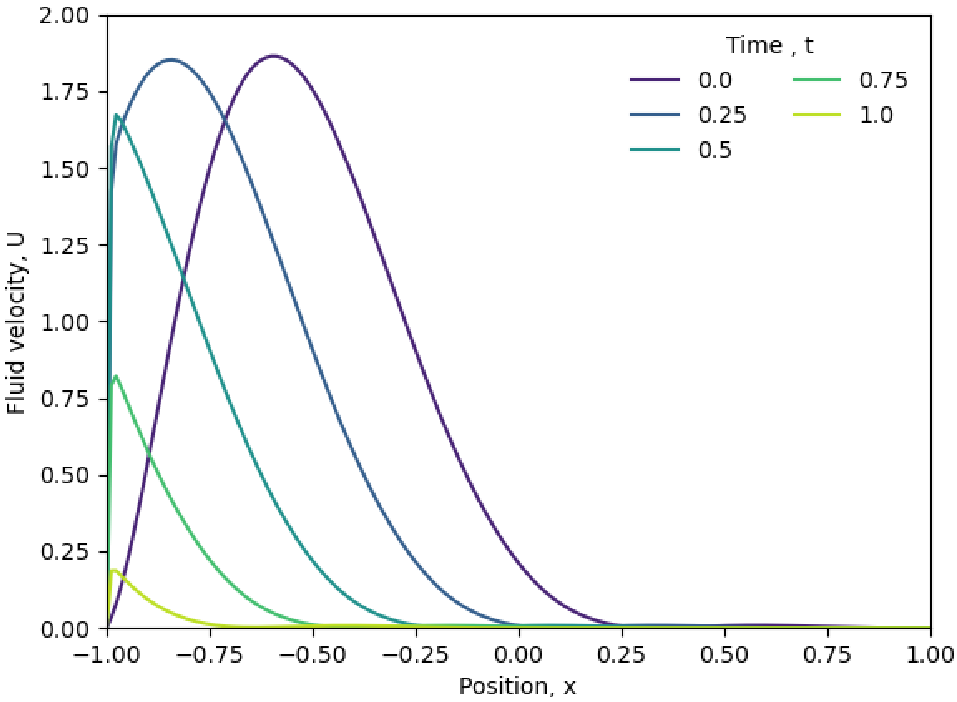


Figure 11: A plot of position vs velocity for ϑ=0.0, μ= 76.56 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

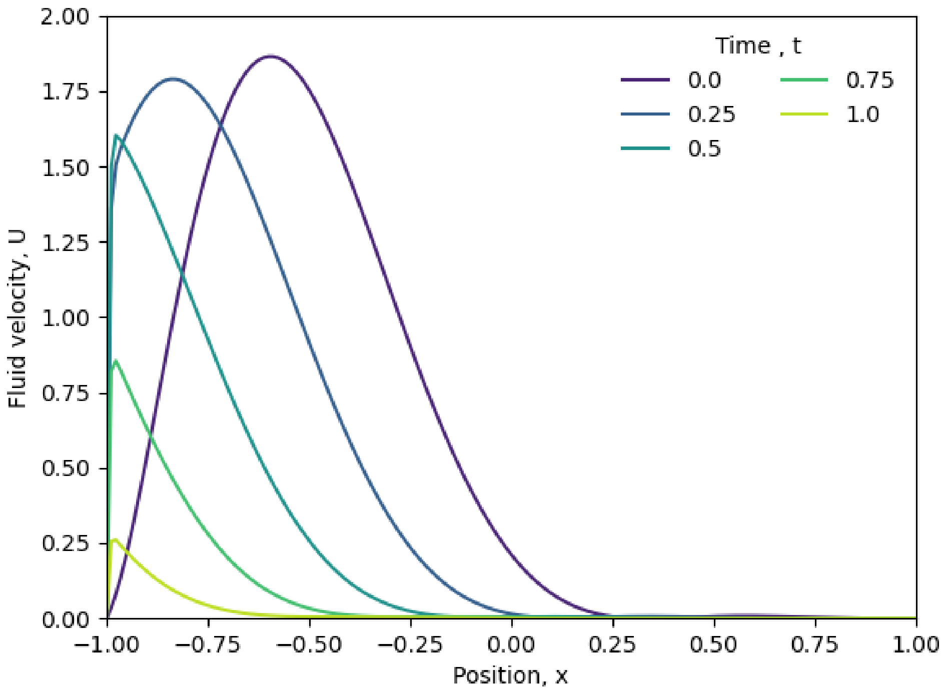


Figure 12: A plot of position vs velocity for ϑ=1.0, μ= 76.56 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

6 continued) The stability/instability condition is defined by the following equation

$$-a_j e^{-ik\Delta x}\lambda + b_j\lambda - c_j e^{ik\Delta x}\lambda = \varepsilon(1-\theta)e^{-ik\Delta x} + 1 + \mu(1-\theta)(-2\varepsilon-\Delta x a^n) + \mu(1-\theta)\left[\varepsilon e^{ik\Delta x} + \Delta x a^n e^{ik\Delta x}\right]$$

~~to~~ The where $a_j = \mu\varepsilon\theta$, $b_j = 1+\mu\theta(2\varepsilon + a^{n+1}\Delta x)$

$c_j = \mu\theta(\varepsilon + a^{n+1}\Delta x)$

~~you~~ this yields

$$\lambda = \frac{\varepsilon(1-\theta)e^{-ik\Delta x} + 1 + \mu(1-\theta)(-2\varepsilon-\Delta x a^n) + \mu(1-\theta)\left[\varepsilon e^{ik\Delta x} + \Delta x a^n e^{ik\Delta x}\right]}{-a_j e^{-ik\Delta x} + b_j - c_j e^{ik\Delta x}}$$

~~so~~ the stability criterion is $|\lambda| \leq 1$ so you would set $|\lambda| = 1$ to find the onset of stability ~~by using gradient desce~~ and solve this equation. You would also follow a similar process for the maximum theorem.

When $\theta = 1$; $\lambda = \dfrac{\varepsilon(0)e^{-ik\Delta x} + 1 + 0[\;''\;''\;] + 0[\;''\;]}{0 + 1 + 0 + 0}$

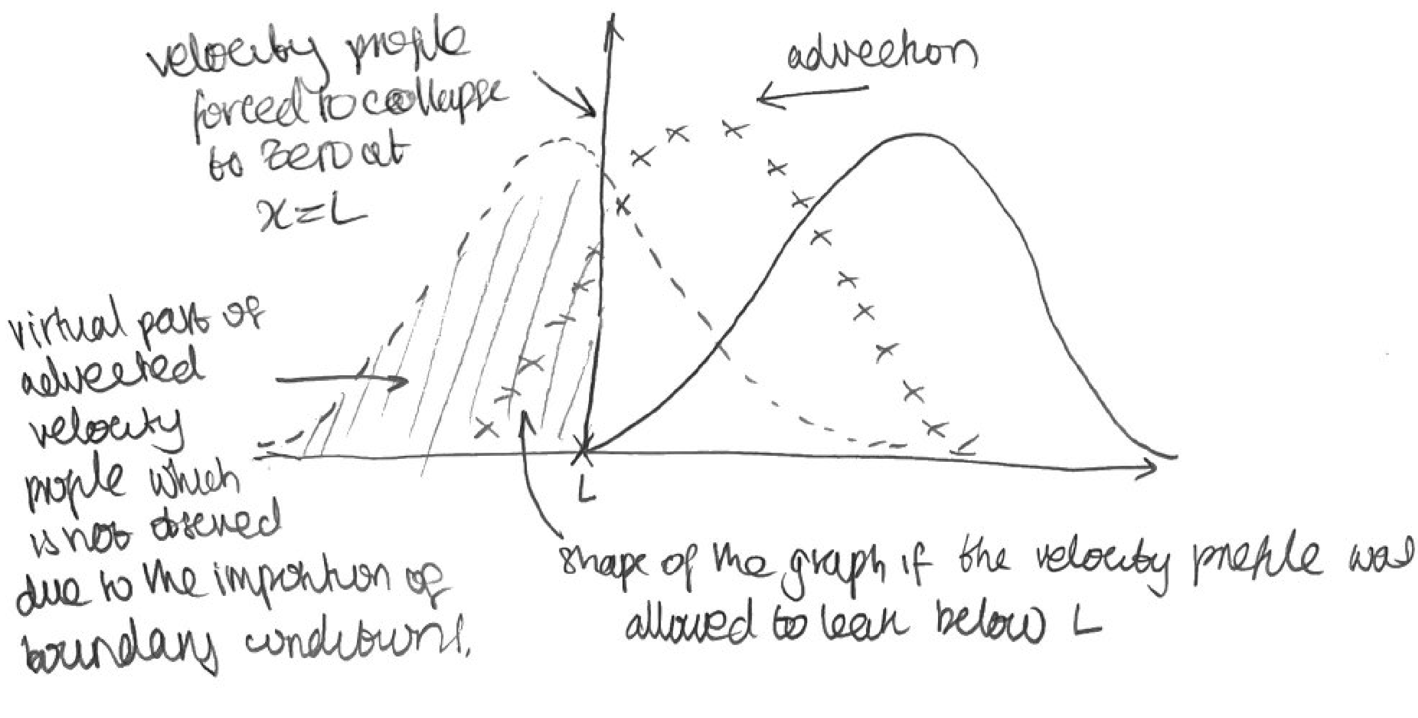
$= 1$

$\therefore \lambda^n = 1^n = 1$ for all values of n. This means that there is no amplitude error, meaning that this choice seems necessary to minimise the error within the simulation and for the solution to correctly converge.

7) Like in Q6, the np.random seed was set to 11. This gave b_k values of [0.18026969, 0.01947524, 0.46321853, 0.72493393]. ~~The Figures~~

~~A The :~~ To generate Figures ~~15-19~~ 13-17, the timestep dt was set to 0.01 and dx was varied ~~to~~ from 0.1 to 1.0×10^{-5} in powers of ten. It is clear to see that refining dx greatly ~~impro~~ improved the quality of the results near $x=-1$. By reducing dx, the position of the peaks shifted towards the ~~b~~ wall at $x=-1$. This suggests that the velocity collapses suddenly at the boundary due to the imposition of the ~~B~~boundary condition $u(\cancel{x}-1, t)=0$ for all times t.

It is also interesting to note the general form of the graph in each simulation (regardless of resolution). As the system evolves in time, the ~~wave~~ velocity profile is advected in the $-\hat{x}$ direction until it hits the wall. This causes a local maxima to develop near $x=-1$ which is observed within all of the graphs ~~at t=0,~~ from $t=0.5$. The magnitude of this peak then collapses as a function of time ~~as~~ due to diffusion, and the fact that the true advected wave profile is further in the $-\hat{x}$ direction.



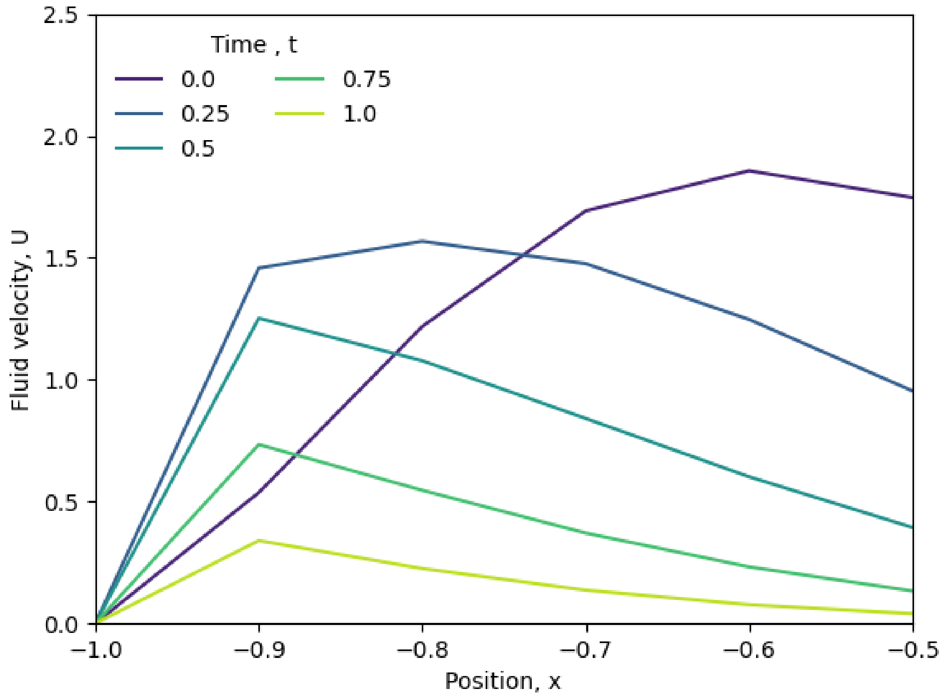


Figure 13: Velocity against position for dx=0.1, dt=0.01, ϑ=1.0 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

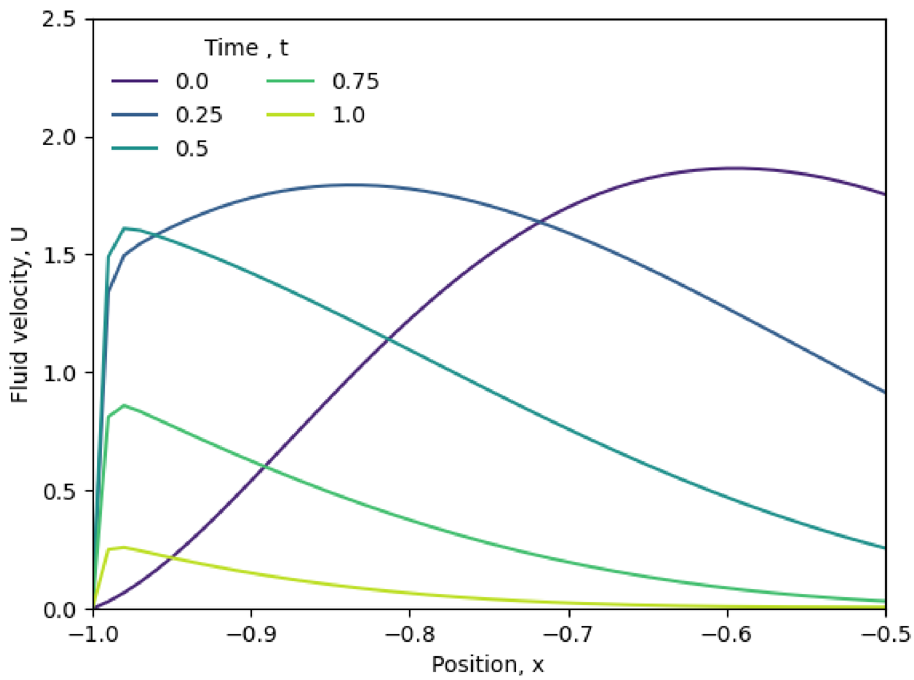


Figure 14: Velocity against position for dx=0.01, ϑ=1.0, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

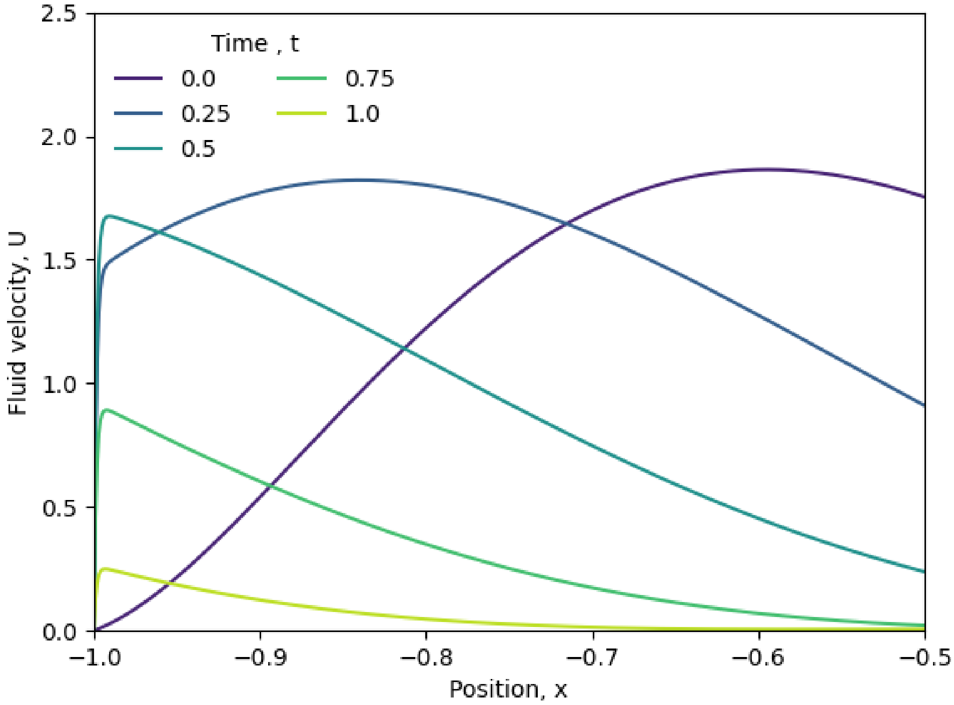


Figure 15: Velocity against position for dx=0.001, ϑ=1.0, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

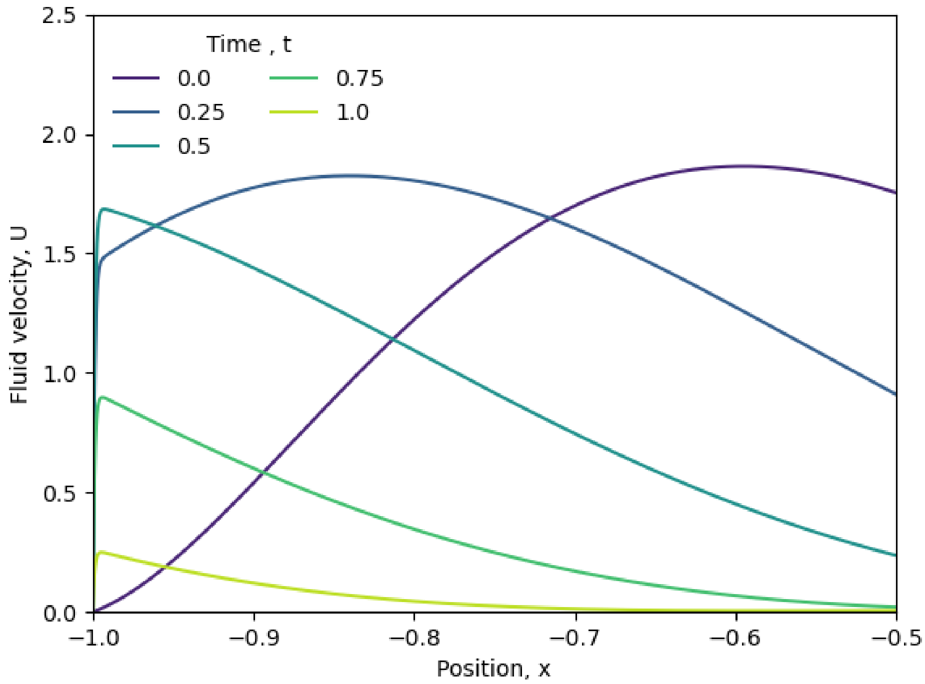


Figure 16: Velocity against position for dx=0.0001, ϑ=1.0, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

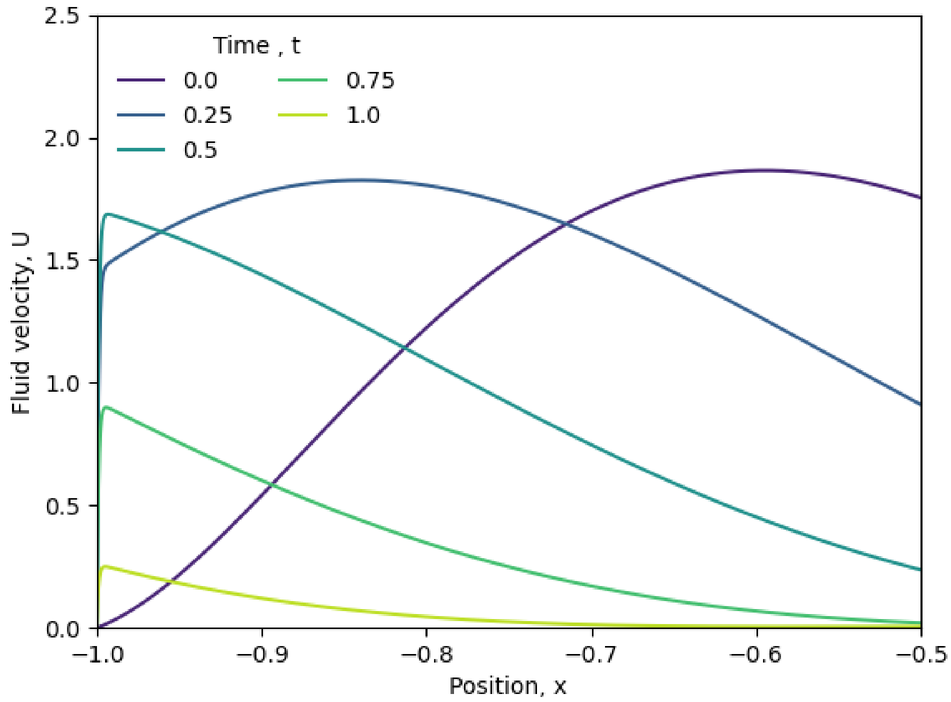
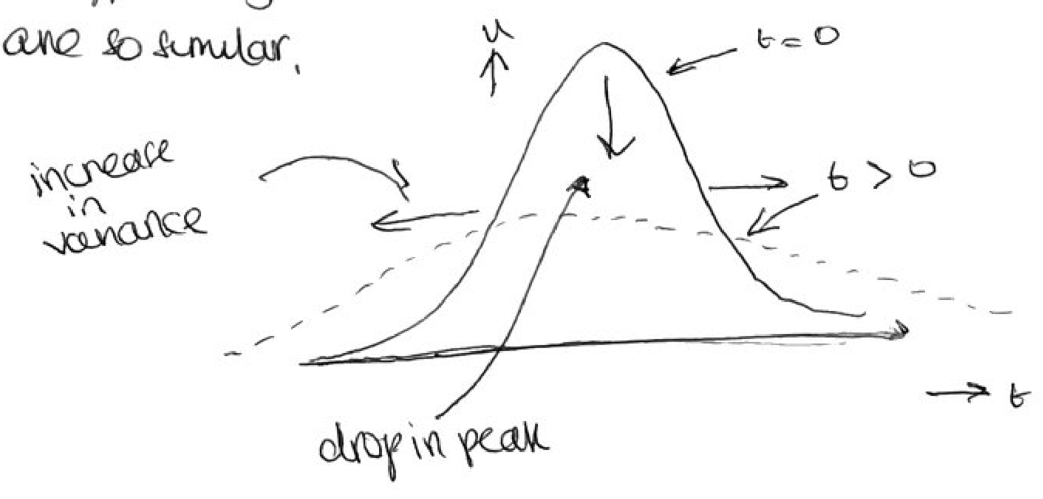


Figure 17: Velocity against position for dx=0.00001, ϑ=1.0, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k \varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

8)

Figures 18 – 20 show how varying ε when $a=1$ affects the profile of the velocity curves. Like before, the timestep dt was set to 0.01 and ~~dx was varied from set to 0.0001~~ the b_k values were [0.1806269 69, 0.01947524, 0.46321853, 0.72493393]. dx was set to 1×10^{-4} as this still ran relatively quickly yet preserved accuracy. ε was varied from 1×10^{-4} to 1×10^{-6} in powers of ten. Since ε was already very small, varying it appeared to have little effect on the profile of the curves. Rather, advection appeared to be the main factor which affected the magnitude of the velocity profiles at ~~its peaks~~ their peaks.

To further explore the effect of diffusion on the velocity profiles, a was set to 0 and ε was varied from 1×10^{-3} – 1 in powers of ten to produce Figures 21 – 24. All of the other parameters were ~~the same as the~~ set to the same values as before. ~~Now,~~ By turning off advection, it was clear that ~~increasing ε can have~~ changing ε can greatly affect the spread and velocity maxima of the curves. ~~Past $\varepsilon = 1\times10^{-3}$, diffusion appears to play a negligible effect~~ However, below $\varepsilon = 1\times10^{-3}$, diffusion is effectively turned off which explains why Figures 18 – 20 are so similar.



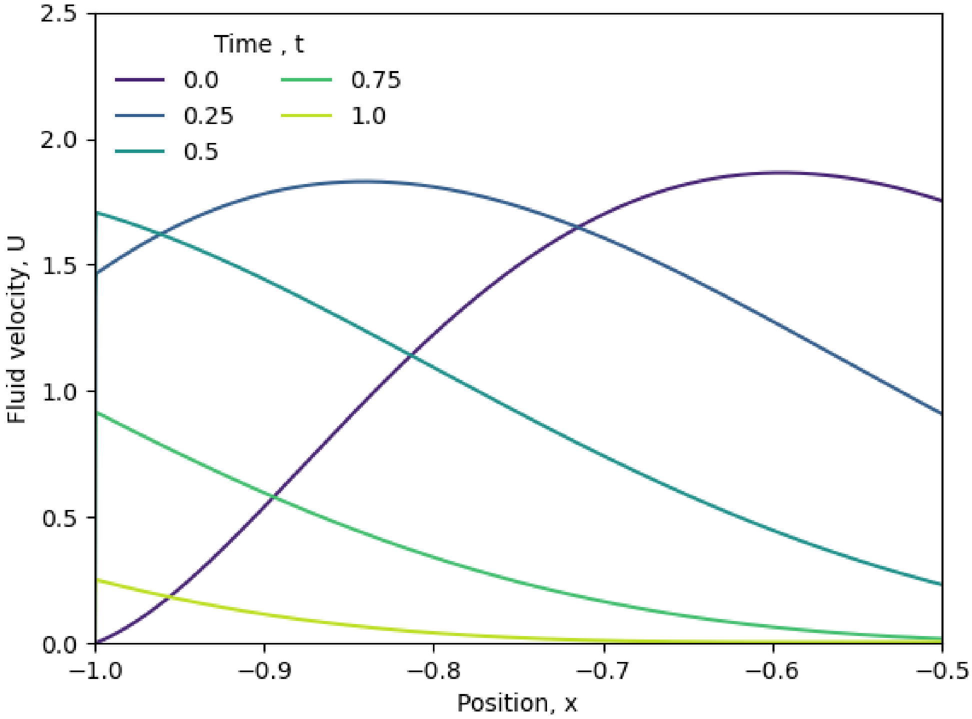


Figure 18: Velocity against position for dx=0.0001, ϑ=1.0, ε=1x10^-4, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

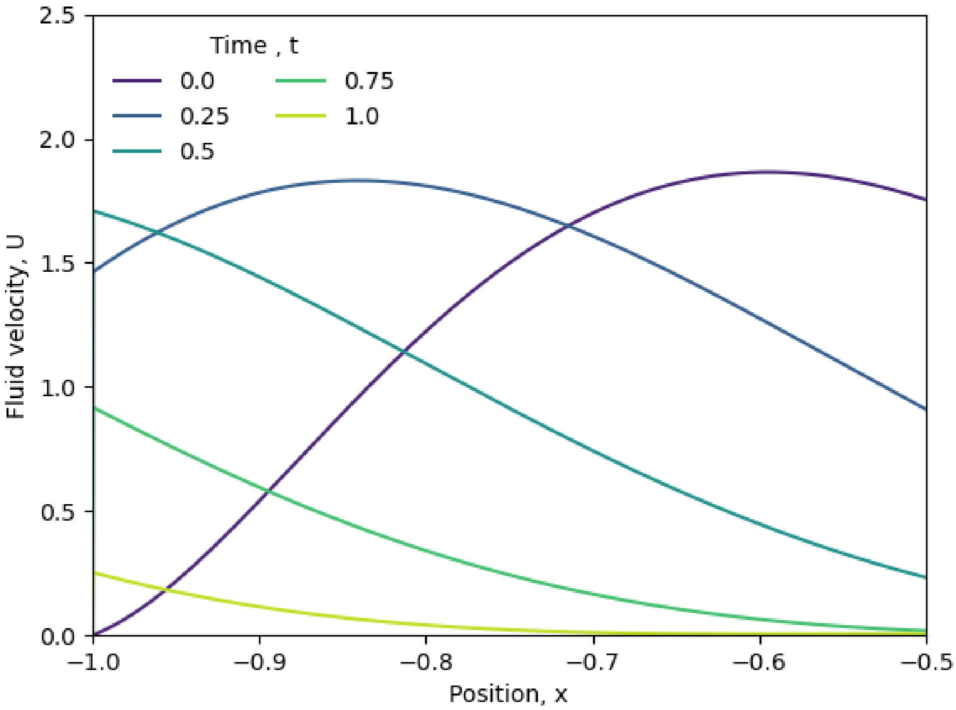


Figure 19: Velocity against position for dx=0.0001, ϑ=1.0, ε=1x10^-5, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

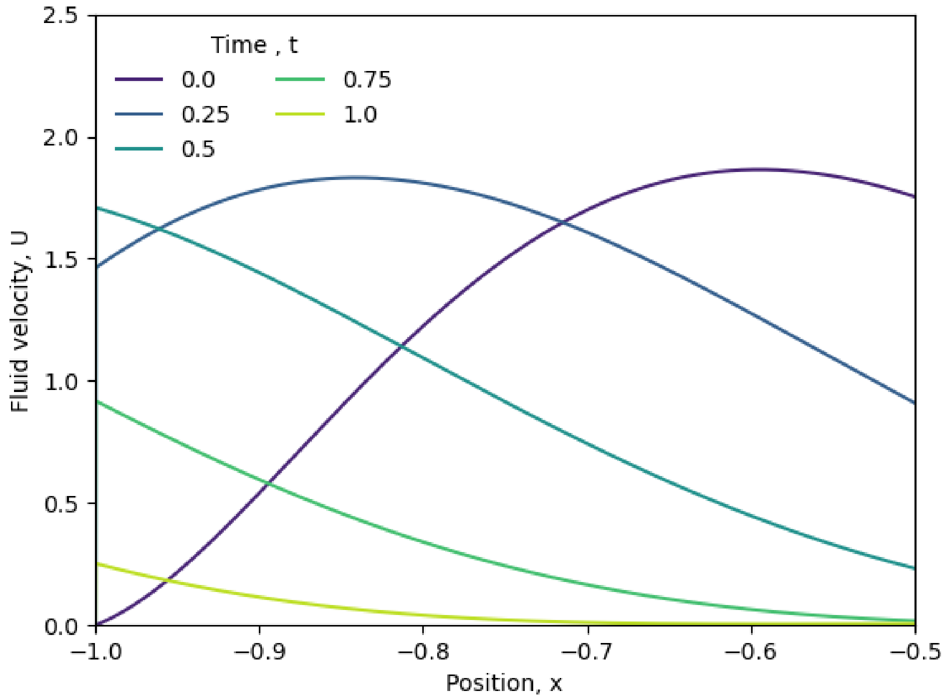


Figure 20: Velocity against position for dx=0.0001, ϑ=1.0, ε=1x10^-6, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials.*

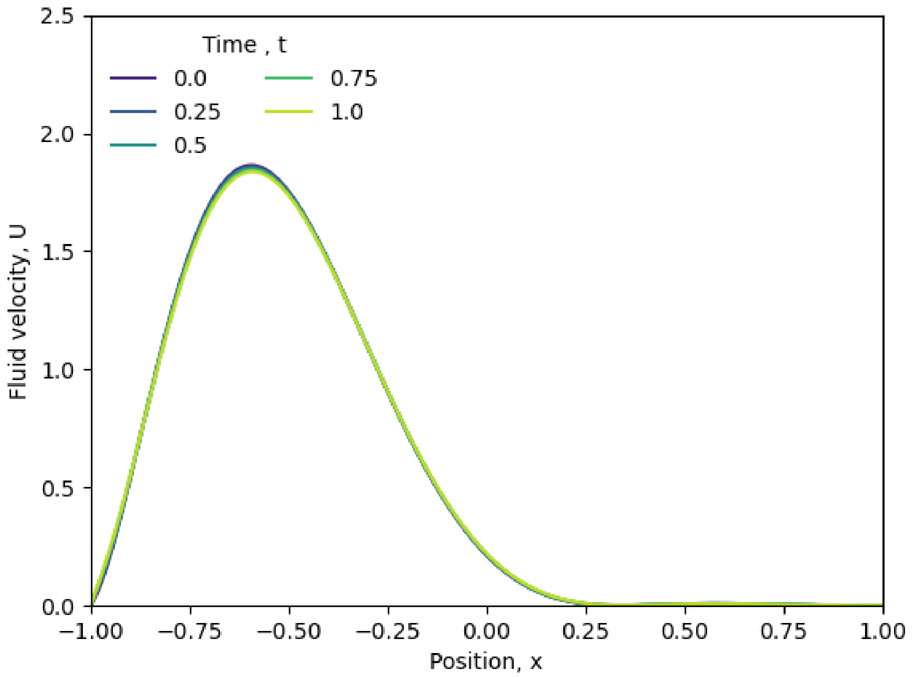


Figure 21: Velocity against position for dx=0.0001, ϑ=1.0, ε=1x10^-3, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials. Here, a has been set to 1 so that the effect of changing the diffusion coefficient can be easily observed.*

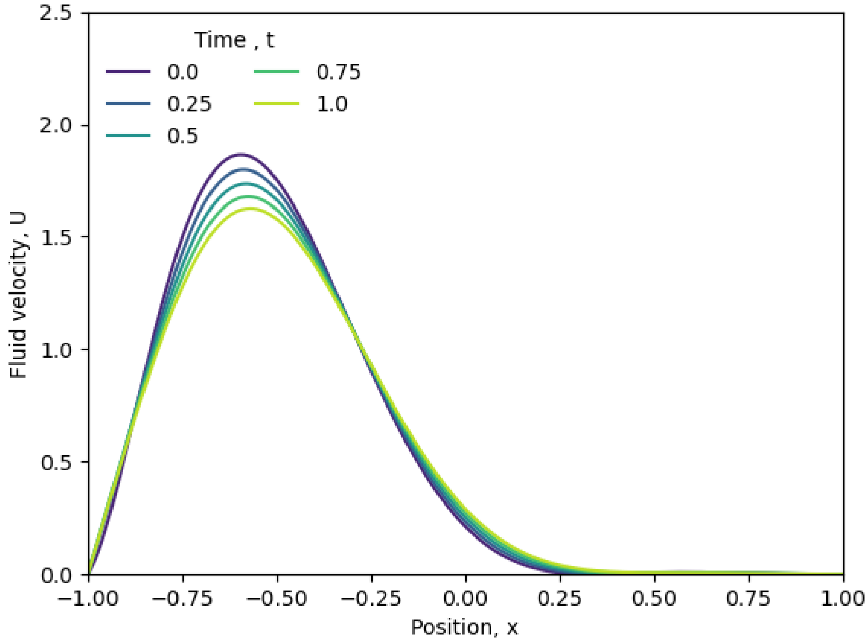


Figure 22: Velocity against position for dx=0.0001, ϑ=1.0, ε=1x10^-2, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k \varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials. Here, a has been set to 1 so that the effect of changing the diffusion coefficient can be easily observed.*

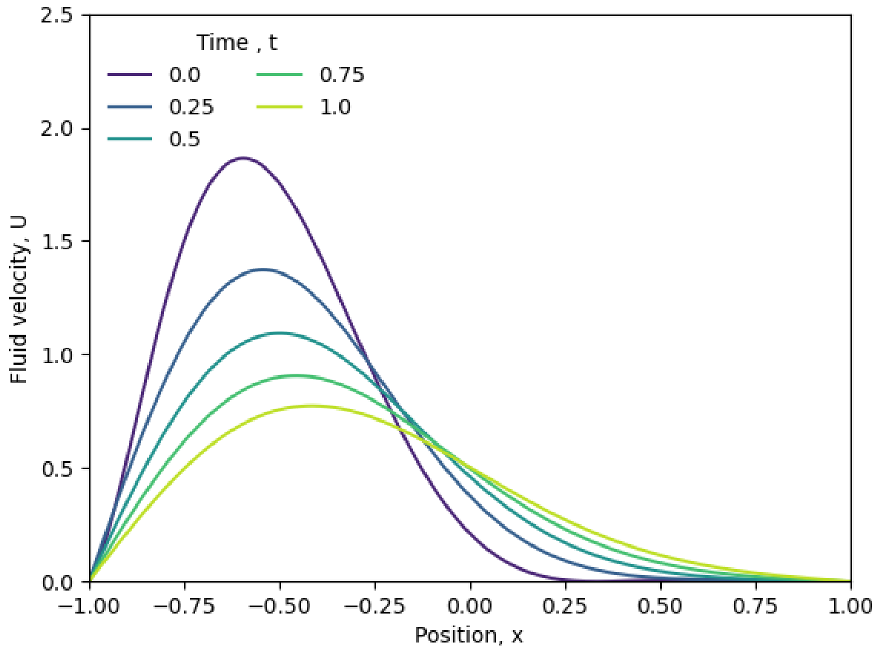


Figure 23: Velocity against position for dx=0.0001, ϑ=1.0, ε=1x10^-1, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k \varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials. Here, a has been set to 1 so that the effect of changing the diffusion coefficient can be easily observed.*

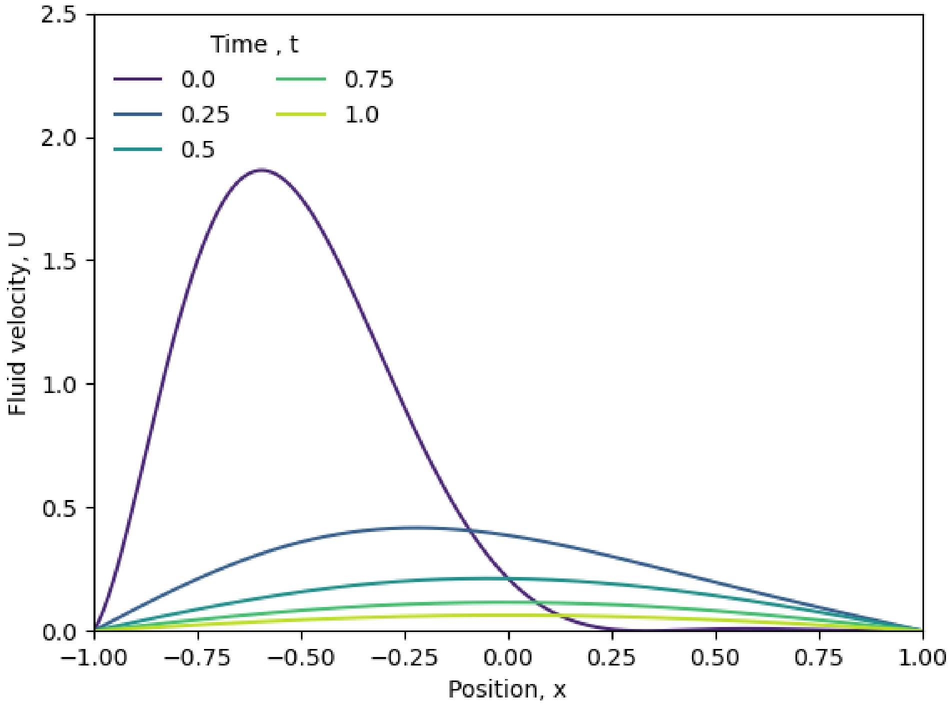


Figure 24: Velocity against position for dx=0.0001, ϑ=1.0, ε=1x10⁻³, dt=0.01 and $u(x,0) = (1-x)^4(1+x)\left(\sum_{k=0}^{3} b_k\varphi_k + C\right)$ *where* φ_k *are the Legendre polynomials. Here, a has been set to 1 so that the effect of changing the diffusion coefficient can be easily observed.*