Numerical Methods Assignment 1

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1 Theory questions

1.
Advection is the transport of the fluid's properties, e.g. some fine particle suspended in the fluid, via the overall motion of the fluid. It can also refer to the transport of the fluid itself due to a component of its own momentum.

Diffusion if the process by which concentration gradients are equalised. In the case of a fluid, it would cause an initial high concentration of fine particles suspended in the liquid to spread out until they are equally concentrated throughout the liquid. In a fluid we can also think of diffusion in terms of the fluid velocities, which will themselves equalise over time.

A linear relationship is one in which a changes in the input create changes changes in the output which only scale according to some constant factor, for example $y = Cx$. Importantly Δy is constant in response to equally sized $Deltax$. This compares to a non-linear example such as higher order polynomials where Δy scales with the input.

The equation is a linear advection-diffusion equation because:

1. Each term has only first power exponents, and there are no non-linear functions such as exponential, so the overall equation is linear.
2. The u_x term describes how the velocity changes with respect to position. The spacial non-uniformity of the velocity (ie. $u_x \neq 0$) provides advection, as some parts of fluid are moving relative to others.
3. The $u_x x$ term describes how the above terms evolves when differentiated again over the spacial the domain. This causes a diffusion effect in the velocity.

2.

$$U_j^{n+1} = [U + \frac{1}{2}\Delta t U_t + \frac{1}{2}(\frac{1}{2}\Delta t)^2 U_{tt} + \frac{1}{6}(\frac{1}{2}\Delta t)^3 U_{ttt} + \cdots]$$

$$U_j^n = [U - \frac{1}{2}\Delta t U_t + \frac{1}{2}(\frac{1}{2}\Delta t)^2 U_{tt} - \frac{1}{6}(\frac{1}{2}\Delta t)^3 U_{ttt} + \cdots]$$

$$(U_j^{n+1} - U_j^n)_{even} = [(U - U) + (\frac{1}{2}(\frac{1}{2}\Delta t)^2 U_{tt} - \frac{1}{2}(\frac{1}{2}\Delta t)^2 U_{tt}) + \cdots] = 0$$

$$(U_j^{n+1} - U_j^n)_{odd} = [(\frac{1}{2}\Delta t U_t + (\frac{1}{2}\Delta t U_t) + \frac{1}{6}(\frac{1}{2})^3 (\Delta t)^3 U_{ttt} + \cdots] = [(\frac{1}{2}\Delta t U_t + (\frac{1}{2}\Delta t U_t) + (\frac{1}{24})(\Delta t) + \cdots]$$

Therefore as in 2.80:

$$U_j^{n+1} - U_j^n = \delta_t U_j^{n+\frac{1}{2}} = [\Delta t U_t + \frac{1}{24}(\Delta t)^3 U_{ttt} + \cdots]$$

Then, using

$$\delta_x^2 U_j^{n+1} = [(\Delta x)^2 U_{xx} + \frac{1}{12}(\Delta x)^4 U_{xxxx} + \frac{2}{6!}(\Delta x)^6 U_{xxxxxx} + \cdots]_j^{n+1}$$

expanded at $(x_j, t_{n+\frac{1}{2}})$

$$\theta \delta_x^2 U_j^{n+1} = \theta f(t + \frac{\Delta}{2}) = \theta[(\Delta x)^2 U_{xx} + \frac{1}{12}(\Delta x)^4 U_{xxxx} + \cdots] + \theta \frac{\Delta}{2}[\Delta x)^2 U_{xxt} + \frac{1}{12}(\Delta x)^4 U_{xxxxt} + \cdots] + \frac{\theta}{2}(\frac{\Delta t}{2})^2 [\Delta x)^2 U_{xxtt} + \frac{1}{12}(\Delta x)^4 U_{xxxxtt} + \cdots]$$

Similarly

$$(1-\theta)\delta_x^2 U_j^n = (1-\theta) f(t + \frac{\Delta}{2}) = (1-\theta)[(\Delta x)^2 u_{xx} + \frac{1}{12}(\Delta x)^4 U_{xxxx} + \cdots] - (1-\theta)\frac{\Delta}{2}[\Delta x)^2 u_{xxt} + \frac{1}{12}(\Delta x)^4 U_{xxxxt} + \cdots] + \frac{(1-\theta)}{2}(\frac{\Delta t}{2})^2 [\Delta x)^2 u_{xxtt} + \frac{1}{12}(\Delta x)^4 U_{xxxxtt} + \cdots]$$

We have terms:

$$(\theta \delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n)_{even} = [(\Delta x)^2 u_{xx} + \frac{1}{12}(\Delta x)^4 U_{xxxx} + \cdots] + \frac{1}{2}(\frac{\Delta t}{2})^2 [\Delta x)^2 u_{xxtt} + \frac{1}{12}(\Delta x)^4 U_{xxxxtt} + \cdots]$$

and

$$(\theta \delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n)_{odd} = 2(\theta - 1)\frac{\Delta}{2}[\Delta x)^2 U_{xxt} + \frac{1}{12}(\Delta x)^4 U_{xxxxt} + \cdots] = (\theta - \frac{1}{2})\Delta t[\Delta x)^2 U_{xxt} + \frac{1}{12}(\Delta x)^4 U_{xxxxt} + \cdots]$$

Therefore as in 2.82.

$$\theta \delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n = [(\Delta x)^2 u_{xx} + \frac{1}{12}(\Delta x)^4 U_{xxxx} + \cdots] + (\theta - \frac{1}{2})\Delta t[(\Delta x)^2 u_{xxt} + \frac{1}{12}(\Delta x)^4 U_{xxxxt} + \cdots] + \frac{1}{8}(\Delta t)^2 (\Delta x^2)[(u_{xxtt} + \frac{1}{12}(\Delta x)^2 U_{xxxxtt} + \cdots]$$

$$\frac{\theta\Delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n}{(\Delta x)^2} = [U_{xx} + \frac{1}{12}(\Delta x)^2 U_{xxxx} + \cdots] + (\theta - \frac{1}{2})\Delta t[U_{xxt} + \frac{1}{12}(\Delta x)^2 U_{xxxxt} + \cdots] + \frac{1}{8}(\Delta t)^2[(U_{xxtt} + \frac{1}{12}(\Delta x)^2 U_{xxxxtt} + \cdots]$$

$$\frac{\delta_t U_j^{n+\frac{1}{2}}}{\Delta t} = [U_t + \frac{1}{24}(\Delta t)^2 U_{ttt} + \cdots]$$

Therefore

$$\frac{\delta_t U_j^{n+\frac{1}{2}}}{\Delta t} - \frac{\theta\Delta_x^2 U_j^{n+1} + (1-\theta)\delta_x^2 U_j^n}{(\Delta x)^2} = U_t - U_{xx} + \frac{1}{24}(\Delta t)^2 U_{ttt} - \frac{1}{12} U_{xxxx} +$$

$$(\frac{1}{2} - \theta)\Delta t[U_{xxt} + \frac{1}{12}(\Delta x)^2 U_{xxxxt} + \cdots] - \frac{1}{8}(\Delta t)^2[U_{xxtt} + \frac{1}{12}(\Delta x)^2 U_{xxxxtt} + \cdots] =$$

$$[u_t - u_{xx}] + [(\frac{1}{2} - \theta)\Delta t U_{xxt} - \frac{1}{12}(\Delta x)^2 U_{xxxx}] + [\frac{1}{24}(\Delta t)^2 U_{ttt} - \frac{1}{8}(\Delta t)^2 U_{xxtt}] + [\frac{1}{12}(\frac{1}{2} - \theta)\Delta t(\Delta x)^2 Uxxxxt + \cdots]$$

3. With the scheme $j = 0, 1, 2...J$, $t = 0, 1, 2, ...$

$$u_t = \frac{u_j^{n+1} - u_j^n}{\Delta t}$$

For u_{xx} take the theta weighted average of second centred difference of

$$u_{xx}(x_j, t^{n+1})$$

and

$$u_{xx}(x_j, t^n)$$

[**?**]

$$\epsilon u_{xx} \approx \frac{\epsilon}{(\Delta x)^2}[\theta(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) + (1-\theta)(U_{j+1}^n - 2U_j^n + U_{j-1}^n)]$$

Therefore, the scheme can be written as:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \theta f(U_j^{n+1}) + (1-\theta) f(U_j^n) + \frac{\epsilon}{(\Delta x)^2}[\theta(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) + (1-\theta)(U_{j+1}^n - 2U_j^n + U_{j-1}^n)]$$

Where $f = a(t)u_x$.
Using a first order upwind discretisation for f we obtain:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = -\frac{1}{\Delta x}[\theta(a^+ U_x^{n+1^-} + a^- U_x^{n+1^+}) + (1-\theta)(a^+ U_x^{n^-} + a^- U_x^{n^+})]$$

where

$$a^+ = max(a,0), a^- = min(a,0)$$

$$U_x^{n^-} = U_j^n - U_{j-1}^n$$

$$U_x^{n^+} = U_{j+1}^n - U_j^n$$

$$U_x^{n+1^-} = U_j^{n+1} - U_{j-1}^{n+1}$$

$$U_x^{n+1^+} = U_{j+1}^{n+1} - U_j^{n+1}$$

Giving a final scheme

$$U_j^{n+1} - U_j^n = -\frac{\Delta t}{\Delta x}[\theta(a^+ U_x^{n+1^-} + a^- U_x^{n+1^+} + (1-\theta)(a^+ U_x^{n^-} + a^- U_x^{n^+})] + \frac{\epsilon \Delta t}{(\Delta x)^2}[\theta(U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) + (1-\theta)(U_{j+1}^n - 2U_j^n + U_{j-1}^n)]$$

Grouping known and unknown terms

$$U_j^{n+1} + \frac{\Delta t}{\Delta x}[(\theta)(a^+ U_x^{n+1^-} + a^- U_x^{n+1^+}] - \frac{\epsilon \Delta t}{(\Delta x)^2}[(\theta)](U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}) =$$

$$U_j^n + \frac{\epsilon \Delta t}{(\Delta x)^2}[(1-\theta)(U_{j+1}^n - 2U_j^n + U_{j-1}^n)] + \frac{\Delta t}{\Delta x}[(1-\theta)(a^+ U_x^{n^-} + a^- U_x^{n^+})]$$

Giving the matrix vector form

$$Ab = x$$

where

$$A_{j,j-1} = -\frac{a^+ \theta \Delta t}{\Delta x} - \frac{\epsilon \theta \Delta t}{(\Delta x)^2}$$

$$A_{j,j} = 1 + \frac{2\epsilon \theta \Delta t}{(\Delta x)^2} + \frac{a^+ \theta \Delta t}{\Delta x} - \frac{a^- \theta \Delta t}{\Delta x}$$

$$A_{j,j+1} = \frac{a^+ \theta \Delta t}{\Delta x} - \frac{\epsilon \theta \Delta t}{(\Delta x)^2}$$

$$b[j] = U_j^n + \frac{\epsilon \Delta t}{(\Delta x)^2}[(1-\theta)(U_{j+1}^n - 2U_j^n + U_{j-1}^n)] + \frac{\Delta t}{\Delta x}[(1-\theta)(a^+ U_x^{n^-} + a^- U_x^{n^+})$$

for $1 < j < J-1$.

At the boundary $L_p, j = 0$ and $L, j = J$ we know the values, so:

$$A_{0,0} = 1$$

$$A_{J,J} = 1$$

which will cause the values at b_0 and b_j, which are the boundary conditions, to be moved unchanged into the solution x.

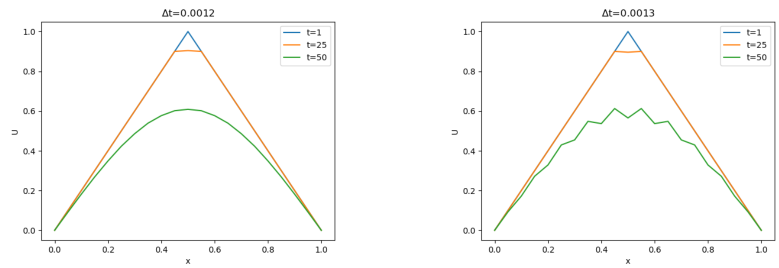

Figure 1: Instability as μ crosses the 0.5 boundary. $\Delta x = 0.05$

4.

The results of the Fourier analysis and Maximum Principle (see Morton-Myers) are: Fourier:

$$e^{-k^2\delta t} = 1 - k^2\delta t + \frac{1}{2}k^4(\Delta t)^2 - \cdots$$

$$\lambda(k) = 1 - 2\mu(\frac{1}{2}(k\Delta x)^2 - \frac{1}{24}(k\delta x)^4 + \cdots) = 1 - k^2\Delta t + \frac{1}{12}k^4\delta t(\delta x)^2$$

Where $\mu = \frac{\delta t}{(\delta x)^2}$

We require for stability that

$$|\lambda(k)| \leq 1 + K\Delta t$$

therefore $\mu \leq \frac{1}{2}$ is stable and $\mu > \frac{1}{2}$ is unstable, assuming $\mu > 0$. This is because λ will grow to negative values with magnitude larger than 1 as μ grows to above 0.5, so we break our stability condition.

Maximum Principle: $\mu \leq \frac{1}{2}$ converges

We can therefore determine that whenever $\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$ the scheme will be stable and converge. When $\frac{\Delta t}{(\Delta x)^2} > \frac{1}{2}$ the scheme will be unstable and will not converge on the solution. We can see this in figure 1. When Δt is 0.0012 $\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}$ and the scheme converges with no instability. When Δt is 0.0013 $\frac{\Delta t}{(\Delta x)^2} > \frac{1}{2}$ and the scheme enters a growing instability which is clearly never going to converge, as the instability will dominate the solution more over time.

5. For the upwind scheme for the $1 - \theta$ part:

When a is positive,

$$\frac{dU_j}{dt} + \frac{(1-\theta)a}{\Delta x}(U_j^n - U_{j-1}^n) = 0$$

Using, where m is the number or waves and L i the length under consideration,

$$U_j(t) = A_m(t)exp(ik_m j\Delta x)$$

$$k_m = \frac{2\pi m}{L}$$

we obtain by substitution

$$\frac{dA_m}{dt}exp(ik_m j\Delta x) + \frac{(1-\theta)a}{\Delta x}[exp(ik_m j\Delta x) - exp(ik_m(j-1)\Delta x)] = 0$$

$$\frac{dA_m}{dt} + \frac{(1-\theta)a\Delta t}{\Delta x}[1 - exp(-ik_m\Delta x)] = 0$$

$$\lambda_m = \frac{-a(1-\theta)\Delta t}{\Delta x}(1 - cos(k_m\Delta x) + isin(k_m\Delta x))$$

When a is negative for the $(1-\theta)$ part:
from

$$\frac{dU_j}{dt} - \frac{(1-\theta)a\Delta t}{\Delta x}(U^n_{j+1} - U^n_j) = 0$$

we obtain

$$\frac{dA_m}{dt}exp(ik_m j\Delta x) - \frac{(1-\theta)a\Delta t}{\Delta x}[exp(ik_m(j+1)\Delta x) - exp(ik_m j\Delta x)] = 0$$

$$\frac{dA_m}{dt} - \frac{(1-\theta)a\Delta t}{\Delta x}[exp(ik_m\Delta x) - 1] = 0$$

$$\lambda_m = \frac{a(1-\theta)\Delta t}{\Delta x}(cos(k_m\Delta x) - 1 + isin(k_m\Delta x))$$

In the negative case

$$|\lambda_m| = [(\frac{-a(1-\theta)\Delta t}{\Delta x})^2(cos^2(k_m\Delta x) - 2cos(k_m\Delta x) + sin^2(k_m\Delta x))]^{\frac{1}{2}}$$

$$|\lambda_m| = [(\frac{-a(1-\theta)\Delta t}{\Delta x})^2(1 - 2cos(k_m\Delta x)]^{\frac{1}{2}}$$

worst case when $\theta = 0$ and $1 - 2cos(k_m\Delta x) = 1$

yielding

$$|\lambda_m| \leq \frac{a\Delta t}{\Delta x}$$

which is equal to the CFL condition. So, the upwind advection scheme is only bound by the CFL condition for stability.

NB: I could not work out how to deal with the $U^{n+1}_{j+1}, U^{n+1}_{j-1}$ values in the θ part of the upwind scheme so I have only dealt with the $1-\theta$ part. Would these be equal to λ evaluated at the $j+1, j-1$ points? Could we therefore say they are equal to λ because of symmetry?

Following a similar methodology we find for the remainder of the scheme, from Morton-Myers:

$$\lambda_m = 1 + \frac{\Delta t}{(\Delta x^2)}[(\theta\lambda + (1-\theta))(exp(-ik_m\Delta) - 2 + exp(ik\Delta x))]$$

$$\lambda_m = \frac{1 - 4(1-\theta)\frac{\Delta t}{(\Delta x^2)} sin^2(\frac{k\Delta x}{2})}{1 + 4(\theta)\frac{\Delta t}{(\Delta x^2)} sin^2(\frac{k\Delta x}{2}}$$

The worst case occurs when the sin^2 term is one, so the range of lambda is $-1 \geq \lambda \leq 1$

for the worst case

$$\frac{4\Delta t}{(\Delta x)^2} \geq 2$$

$$\frac{\Delta t}{(\Delta x)^2} \leq \frac{1}{2}(\frac{1}{1-2\theta})$$

is stable. For values $\frac{1}{2} \leq \theta \leq 1$ this resolves to $\frac{\Delta t}{(\Delta x)^2} \leq 0$ is stable, so the scheme is unconditionally stable in this range. For the range $\theta < \frac{1}{2}$ stability is dependant on the above condition.

The maximum principle analysis gives convergence when

$$\frac{\Delta t}{(\Delta x)^2}(1-\theta) \leq \frac{1}{2}$$

The CFL for a 1 dimensional case is

$$C = \frac{u\Delta t}{\Delta x}$$

$$C \leq C_{max}$$

where C_{max} is 1 for an explicit scheme, or higher for an implicit scheme. For a theta scheme we can expect 1 as the worst case due to the mixture of implicit and explicit schemes. For the simple triangle boundary conditions from

Morton-Mayers $u_{max} = 1$ so we need only consider $\frac{\Delta t}{\Delta x} \leq 1$.

Figure 2 shows the output for $\epsilon = 0, a = 0.02$ as the C is taken from 1 to 2.

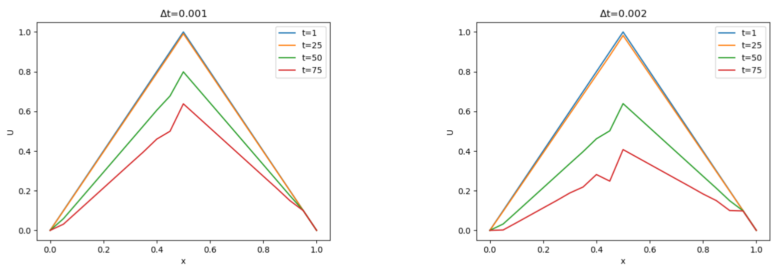

Figure 2: Amplitude collapse as C crosses the 1.0 boundary. $\Delta x = 0.01$

6.

Figures 3 and 4 show the solutions with and without Legendre polynomials for μ 0.1,0.5, and 1. We see that the scheme is stable throughout, but only converges when $\mu \leq 0.5$. Above this value the amplitude collapses too quickly.

We see a similar amplitude pattern in figures 5 and 6 for $\theta = 0.5$. In the case with Legendre polynomials we note that the draw on $\mu = 0.5$ was "unlucky" in the sense that the peak is significantly shifted. This is just an artifact of using random values of b_k.

Finally, we observe that in figures 7 and **??** that when $\theta = 0$ the scheme is unstable and non-convergent. I am not clear on the cause of this as our previous stability analysis would suggest that the scheme should still be conditionally stable and convergent for values $\mu < 0.5$. However, it is clear that choice of $theta = 1$, $\mu \leq 0.5$ would be most appropriate as this is the only scheme with is fully stable and convergent. Any scheme with lower values of θ is averaging an unstable scheme with a stable scheme. It is better to simply use to stable scheme.

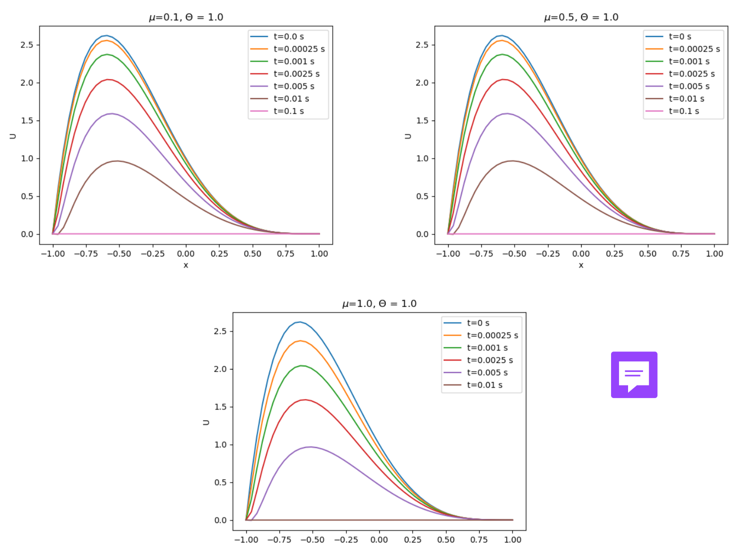

Figure 3: The case for $\theta = 1$ and no Legendre polynomials

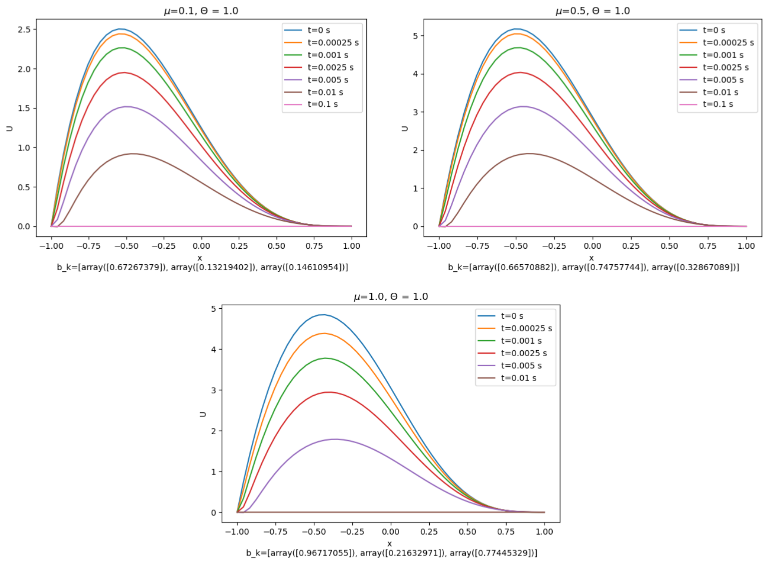

Figure 4: The case for $\theta = 1$ with Legendre polynomials

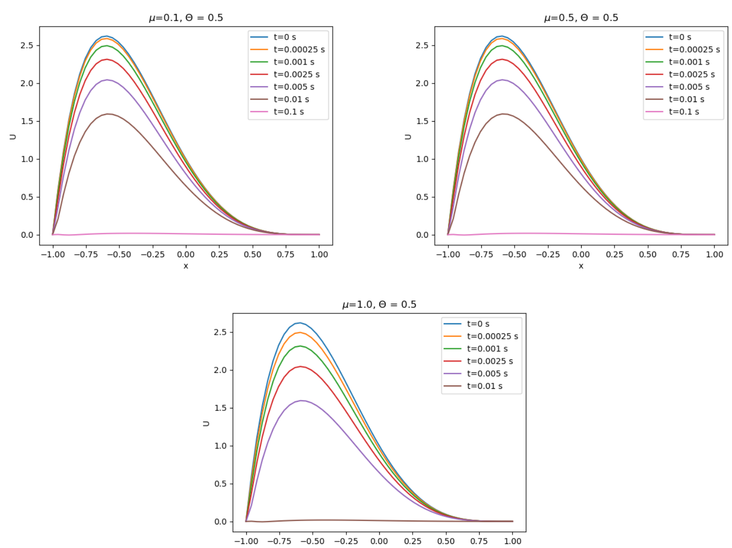

Figure 5: The case for $\theta = 0.5$ and no Legendre polynomials

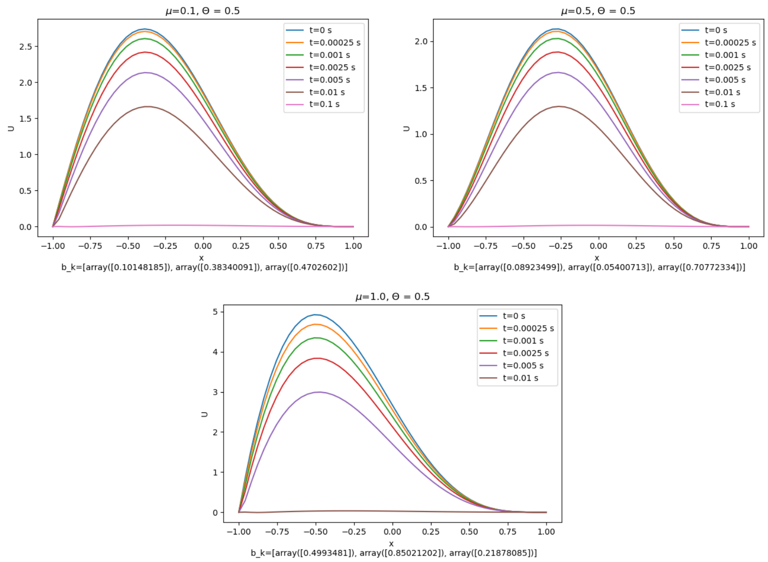

Figure 6: The case for $\theta = 0.5$ with Legendre polynomials

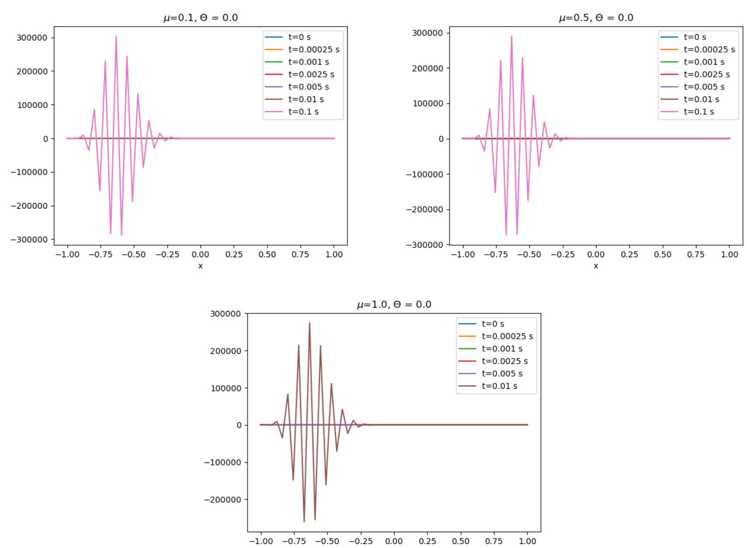

Figure 7: The case for $\theta = 0$ and no Legendre polynomials

7.

We can see in figure 8 that we have not achieved mesh independence for this problem. My code is not fast enough to decrease to Δx any further while maintaining a reasonable value of μ.

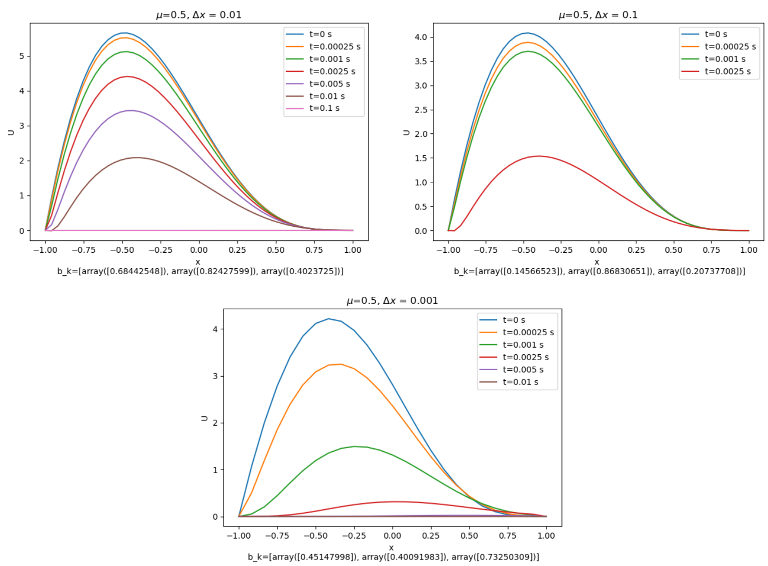

Figure 8: Δx dependence

8.

Figure 9 shows how further reducing the value of ϵ effects the solution. We can observe the peaks are less slightly less diffuse. This is a small effect however, which is not surprising given how reduced the diffusion term is in all cases. The effect is most noticeable near $x = -1$ at early values for t, where we observe that the curve rises more rapidly for lower values of ϵ due to less diffusion.

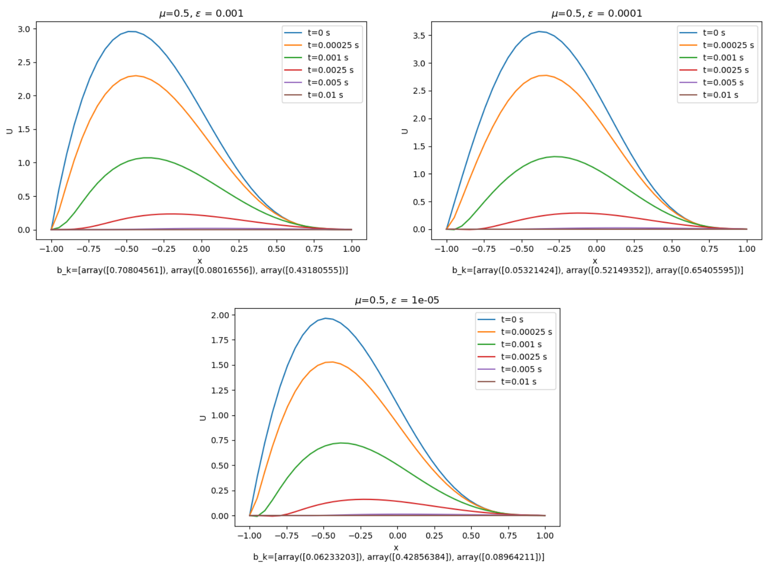

Figure 9: Varying values of ϵ