Numerical Methods Assignment 1

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October 2024

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

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

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

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

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:

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

Where $f = a(t)$ and $a(t) > 1$ for the equation $u - a(t)u_x - \epsilon u_{xx}$. This is achieved simply by taking the explicit equation, multiplied by theta, and adding it to the implicit equation multiplied by theta - 1.

Giving a final scheme

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

Grouping known and unknown terms

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

Giving the matrix vector form

$$Ab = x$$

where

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

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

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

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

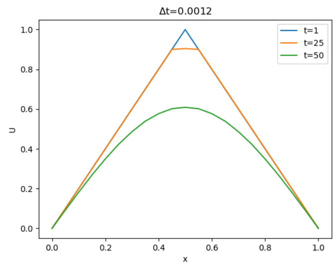
for $1 < j < J - 1$.

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.



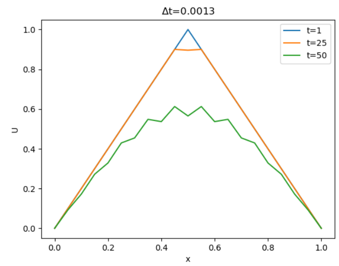


Figure 1: Instability as μ crosses the 0.5 boundary. $\Delta x = 0.05$

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,

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

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

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

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 $U_{j+1}^{n+1}, U_{j-1}^{n+1}$ 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.

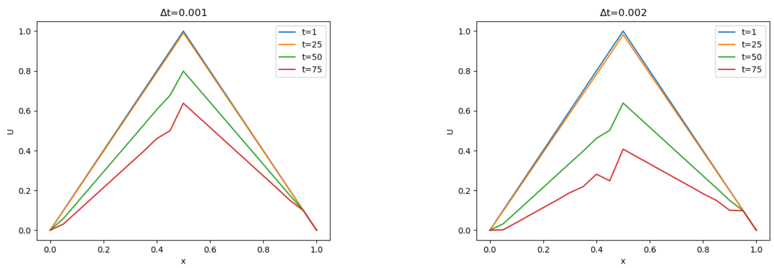
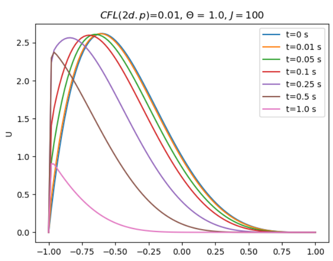


Figure 2: Amplitude collapse as C crosses the 1.0 boundary. $\Delta x = 0.01$

6

Figure 1 shows the implementation of the full scheme ran at values of $t = theta = 1, 0$ with $a = 1$ with boundary condition $u(x, 0) = (1 - x)^4(1 + x)$. We can see that when the scheme meets the CFL condition, $\frac{a\Delta t}{\Delta x} < 1$ both the fully implicit and fully explicit schemes appear to give the same results. Inspection of the resulting arrays in python, by printing the array values to screen, confirm that the results are exactly equal.

When there is no advantage granted by the use of an implicit scheme it is generally preferable to use an explicit scheme as they are faster to calculate. Note, however, that in this implementation the speed gains are lower as we are still solving the system of linear equations. There is a potential speed increase by setting $\theta = 1$, but this is obtained via the sparsity of the b vector which becomes zero everywhere.



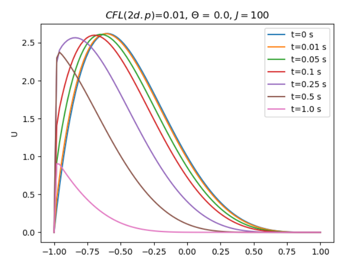


Figure 3 shows what happens if the CFL is raised above 1. The solution becomes unstable with the amplitude collapsing too quickly, this is similar to phenomena observed in figure 2 in question 4.

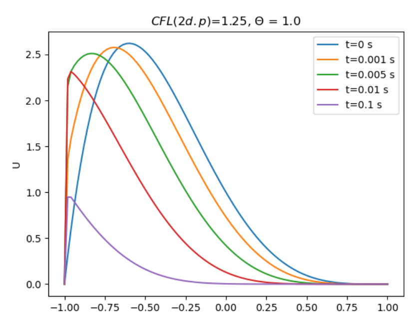


Figure 3: When the CFL condition is violated, the solution becomes unstable

The solution with boundary conditiosn set to be the first three terms of the Legendre polynomial was also implemented, figure **??**. This will be further explored in questions 7 and 8.

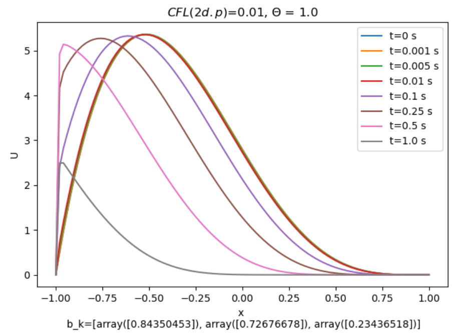


Figure 4: An initial experiment on Legendre polynomials

7

Next, Legendre polynomial was expolred in more detail. We convergence by refining the grid in x. The CLF was mainted at the same value. For this test, fixed values were used for the Legendre polynomials instead of random draws to allow for direct comparisons between grid discretisations.

Figure 5 shows the mesh refinement as we increase the number of grid points from 100 to 400. $\Delta x = \frac{r}{J}$ where r is the size of the computational domain and J is the number of grid points. Therefore, the CFL reduces as J increases. To compensate for this, t is reduced as J is increased to maintain the same CFL. This ensures we are only testing the dependency on the mesh in x, not in time.

The mesh looks like it has become sufficiently refined between 200 and 400 grid points. However, zooming in on the region near the boundary layer (figure 6), shows that there are still differences. Note that the line at $t = 0.5$ changes significantly between $J = 200$ and $J = 400$. Due to computational constraints, higher values of J were not examined.

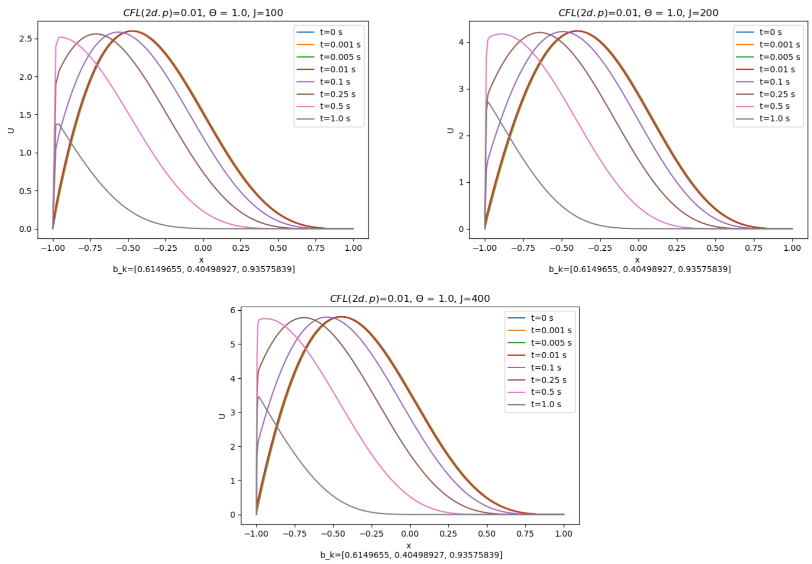


Figure 5: The mesh appears to be becoming refined between J=200 and J=400

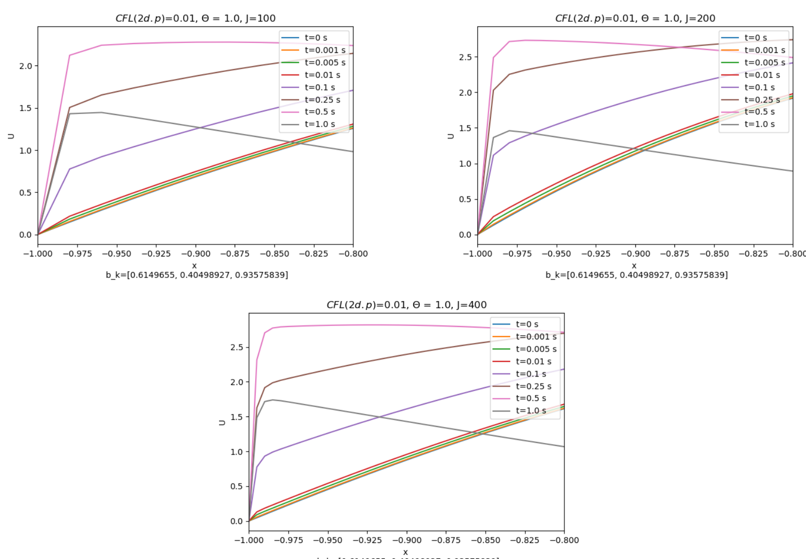


Figure 6: A zoomed in view shows the mesh still isn't fully refined

8

The effect of varying epsilon was examined. Figures 8 and 7 show what happens when epsilon is taken from $\epsilon = 1e^{-}4$ to $\epsilon = 1e^{-}6$. The zoomed out view, figure

7, shows no obvious changes. However, in the zoomed in view (figure 8) we can observe subtle change near the boundary layer. This is particularly visible at $t = 0.5$ and $t = 1.0$. When ϵ is smaller there is a sharper transition from the boundary layer to the rest of the curve. With high $\epsilon = 1e^{-}4$ the transition is smoothed, but as it is decreased the transition occurs suddenly and appear as a discontinuity at this length scale. Zooming in further, combined with a finer grid, should reveal that we are actually shrinking the radius over which the smooth transition occurs.

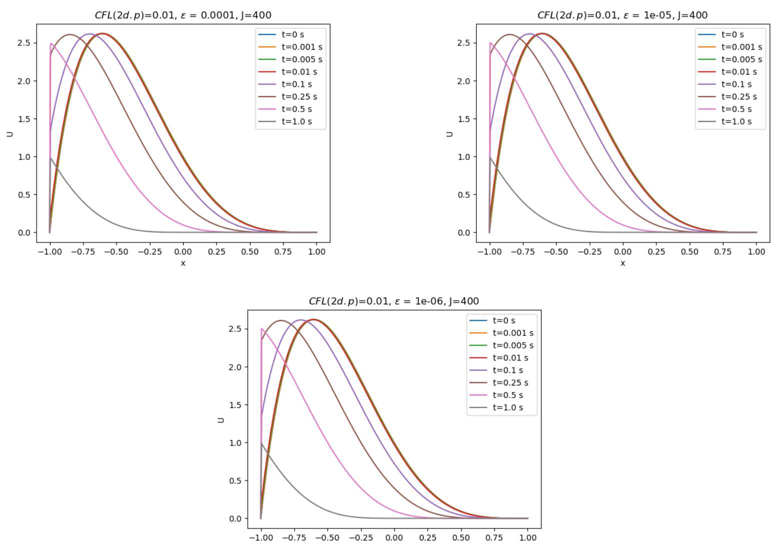


Figure 7: The zoomed out view of changes to ϵ shows no obvious change

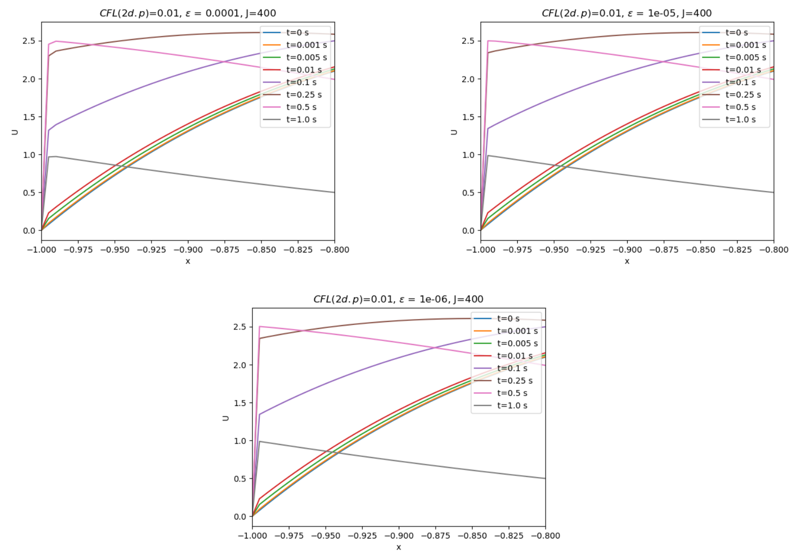


Figure 8: A zoomed in view shows subtle changes at the boundary layer