MATH60025 Computational PDEs Coursework 1

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1 Part A

1.1 1

The steady state solution is $u(x,t) = 0$. This can be found by setting u_t to 0, since the solution shouldn't change in time. This means that $u_{xx} = 0$, meaning that $u(x,t) = ax + b$ for some constants a and b. By applying the boundary conditions, we find that $a = 0$ and $b = 0$, hence the result.

1.2 2

First, assume seperability *i.e.* $u(x,t) = X(x)T(t)$. Then,

$$u_t = X(x)T'(t) \tag{1.1}$$

$$u_{xx} = X''(x)T(t) \tag{1.2}$$

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} \tag{1.3}$$

Since the above holds for all t and x, both sides must be a constant, which we denote λ.

We can then use standard techniques to solve the two ODEs given by

$$T'(t) = \lambda T(t) \tag{1.4}$$

$$X''(x) = \lambda X(x) \tag{1.5}$$

If $\lambda \geq 0$, then the solution to the PDE is

$$u(x,t) = e^{\lambda t}(C_1 \sinh(\sqrt{\lambda}x) + C_2 \cosh(\sqrt{\lambda}x)) \tag{1.6}$$

which we see cannot satisfy the boundary conditions for $t > 0$ unless u is the zero solution. Hence, we consider $\lambda < 0$ instead. The solution is then

$$u(x,t) = e^{\lambda t}(C_1 \sin(\sqrt{-\lambda}x) + C_2 \cos(\sqrt{-\lambda}x)) \tag{1.7}$$

We now find out suitable values for λ that satisfy the boundary conditions. Since $u(0,t) = 0$, we have $C_2 = 0$ and reduce our solution to $Ce^{\lambda t}\sin(\sqrt{-\lambda}x)$, which always satisfies the condition at the boundary $x = 0$. For the other boundary $x = 1$, we need $\sin(\sqrt{-\lambda}) = 0$, resulting in

$$\lambda = -n^2\pi^2 \text{ for } n \in \mathbb{N} \tag{1.8}$$

and solutions $u_n(x,t) = e^{-n^2\pi^2 t}\sin(n\pi x)$.

We will satisfy the initial condition by expanding in a fourier series and superimposing our solutions (as the PDE is linear).

We expand $f(x) = 1$ in terms of a fourier series, whose coefficients a_n can be computed using the inner product

$$a_n = \frac{\int_0^1 f(x)\sin(\pi n x)\,dx}{\int_0^1 \sin(\pi n x)^2\,dx} = \begin{cases} \frac{4}{\pi n} & \text{if } n \text{ is odd} \\ 0 & \text{otherwise} \end{cases} \tag{1.9}$$

We then sum the solutions corresponding to the fourier modes together to get the solution satisfying all the right boundary/initial conditions:

$$u(x,t) = \sum_{k=0}^{\infty} a_k u_k(x,t) = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} e^{-(2n+1)^2\pi^2 t} \sin((2n+1)\pi x) \tag{1.10}$$

1.3 3

We use the finite difference approximations on a mesh with N points in the x direction, with u_n^j denoting the nth point in the direction of x and the jth point in the t direction. We then have

$$\frac{u_n^{j+1} - u_n^j}{k} = \frac{\partial u_n^j}{\partial t} + O(k) \tag{1.11}$$

$$\frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} = \frac{\partial^2 u_n^j}{\partial^2 x} + O(h^2) \tag{1.12}$$

By equating the two derivatives per the PDE, we get the numerical scheme, which has a truncation error that is $O(k)$ and $O(h^2)$.

$$U_n^{j+1} = rU_{n+1}^j + (1-2r)U_n^j + rU_{n-1}^j \tag{1.13}$$

where $r = \frac{k}{h^2}$.

We set all U_0^j and U_N^j to 0 for $j > 0$ and all $U_1^0, \ldots, U_{N-1}^0$ to 1 to encode the boundary conditions.

Relevant code: `q3A`

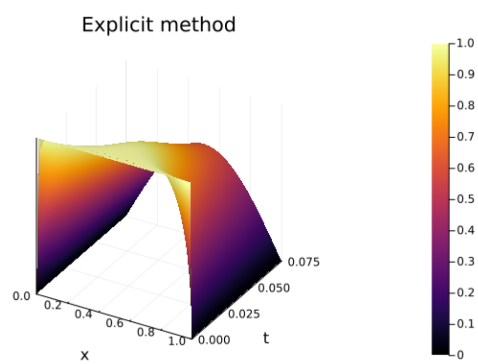
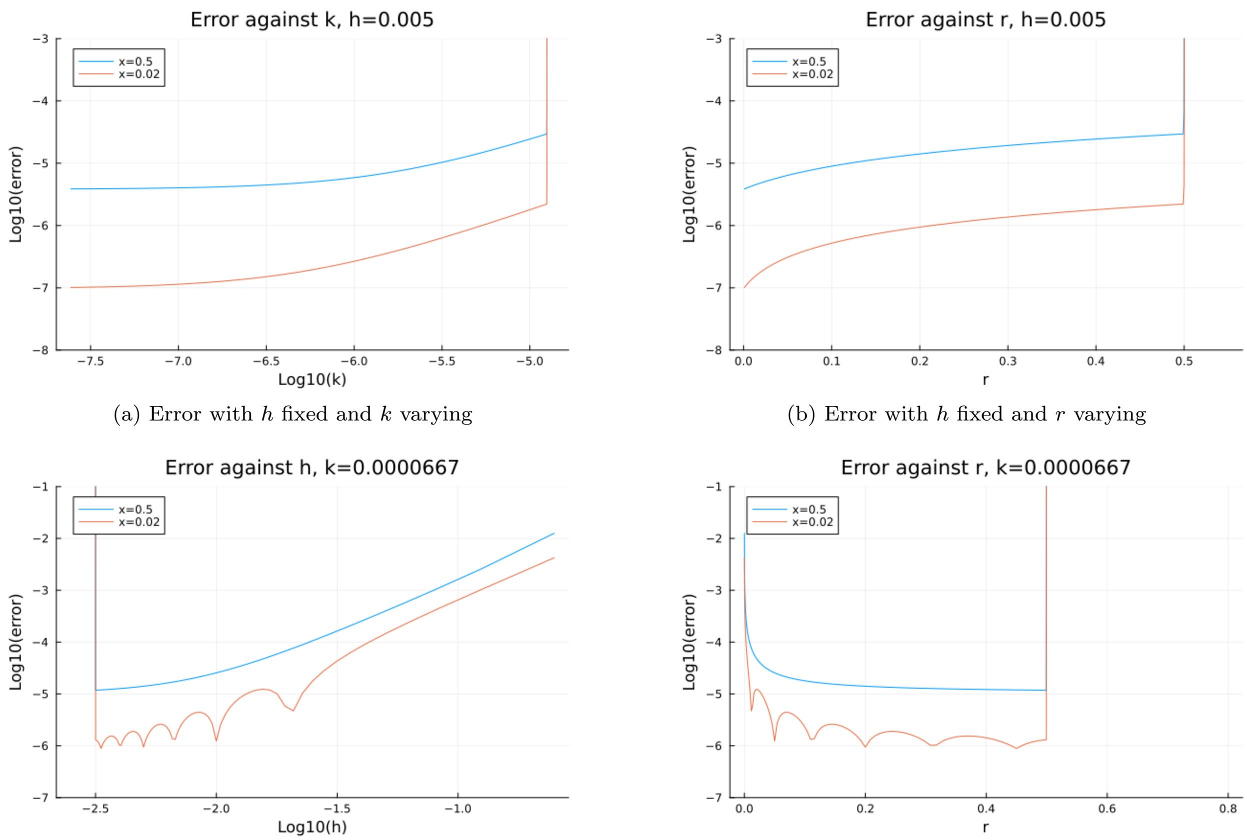


Figure 1: Contour of the solution with the Explicit method on a 101×2001 grid.

1.4 4



(a) Error with h fixed and k varying

(b) Error with h fixed and r varying

(c) Error with k fixed and h varying

(d) Error with k fixed and r varying

Figure 2: Investigation of error with varying h, k and r, at points $x = 0.5$ (Blue) and $x = 0.02$ (Orange).

In Figure 2, we investigate the error of the computed solution and the analytic solution at the points $x = 0.5$ and $x = 0.02$ with $t = 0.075$. In (b) and (d), we see the critical value of $r = 0.5$ where the scheme transitions from stable to unstable.

We see in (a) and (b) that as $k \to 0$, the error is decreasing. In (a), the gradient of the lines near $\log_{10}(k) \approx -5.0$ right hand side is close to 1, reflecting that the truncation error in the scheme is $O(k)$. The leveling off near $\log_{10}(k) \approx -7.5$ is due to the fact that the truncation error is actually $O(k + h^2)$ and the $O(h^2)$ component begins to dominate the truncation error.

Similarly, with (c) we can see that the gradient of the lines is close to 2, reflecting the $O(h^2)$ behaviour of the truncation error. In (d) we see a tradeoff in the value of h. If h is too big, we lose accuracy due to large truncation error, despite the scheme being stable. On the other hand, if h is too small, r becomes bigger than 0.5 and we lose stability.

The error is less at $x = 0.02$ than $x = 0.5$ due to the dependence of the truncation error on x and t. More specifically, the truncation error here is

$$R_n^j = \frac{1}{12} h^2 \frac{\partial^4 u_n^j}{\partial^4 x} - \frac{1}{2} k \frac{\partial^2 u_n^j}{\partial^2 t} + O(k^2, h^4) \tag{1.14}$$

Note that under the assumption of smoothness of the solution, $u_{xxxx} = u_{tt}$. Hence the error is linear in the value of u_{tt} at the point.

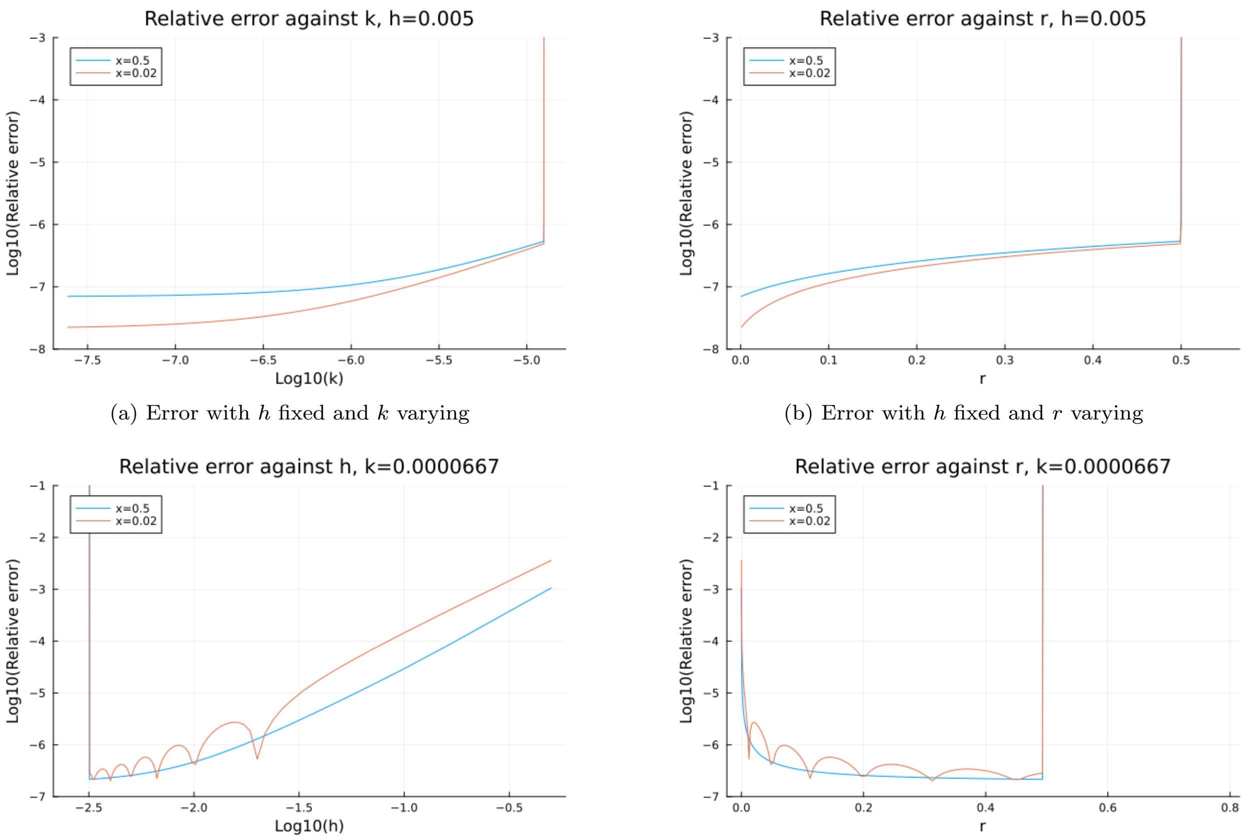
We can calculate u_{tt} using the analytic solution, revealing that $u_{tt}(0.02, 0.075) \approx 4.517$ whilst $u_{tt}(0.5, 0.075) \approx 54.881$. This explains why the error is an order of magnitude higher for $x = 0.5$ than $x = 0.02$.

The weird patterns in the $x = 0.02$ case occur because the number of spacing points N doesn't align with the x value, and instead the calculated value is done via linear interpolation.

1.5 5

We consider measuring log-relative accuracy with respect to u_{tt}, defined as

$$error = \log_{10} \left| \frac{u_{numerical} - u_{analytic}}{u_{tt,analytic}} \right| \tag{1.15}$$



(a) Error with h fixed and k varying

(b) Error with h fixed and r varying

(c) Error with k fixed and h varying

(d) Error with k fixed and r varying

Figure 3: Investigation of relative error with varying h, k and r, at points $x = 0.5$ (Blue) and $x = 0.02$ (Orange).

We see that after rescaling by the partial derivative u_{tt} (which was calculated via the analytic solution), the lines are much closer to each other now and the error for both $x = 0.02$ and $x = 0.5$ behave similarly now, whilst maintaining the features described in the previous question.

1.6 6

The scheme we will be using is described as follows

$$U_n^{j+1} - U_n^j = \frac{r}{2}(\delta^2 U_n^{j+1} + \delta^2 U_n^j) \tag{1.16}$$

which we rearrange into a linear system with tridiagonal matrices as follows

$$U_n^{j+1} - U_n^j = \frac{r}{2}\left(U_{n+1}^{j+1} - 2U_n^{j+1} + U_{n-1}^{j+1} + U_{n+1}^j - 2U_n^j + U_{n-1}^j\right) \tag{1.17}$$

$$
(1+r)\,U_n^{j+1} - \frac{r}{2}U_{n+1}^{j+1} - \frac{r}{2}U_{n-1}^{j+1} = (1-r)\,U_n^j + \frac{r}{2}U_{n+1}^j + \frac{r}{2}U_{n-1}^j \tag{1.18}
$$

resulting in the following system. Here, we are using $U^j = [U_1^j, \ldots, U_{N-1}^j]$

$$
AU^{j+1} = BU^j \tag{1.19}
$$

where

$$
A = \begin{bmatrix} 1+r & -\frac{r}{2} & & \\ -\frac{r}{2} & 1+r & \ddots & \\ & \ddots & \ddots & -\frac{r}{2} \\ & & -\frac{r}{2} & 1+r \end{bmatrix} \qquad B = \begin{bmatrix} 1-r & \frac{r}{2} & & \\ \frac{r}{2} & 1-r & \ddots & \\ & \ddots & \ddots & \frac{r}{2} \\ & & \frac{r}{2} & 1-r \end{bmatrix} \tag{1.20}
$$

Relevant code: `qA6`

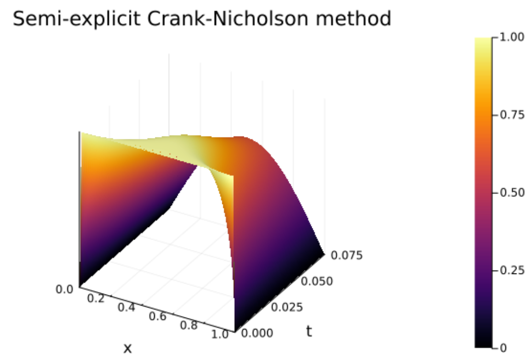
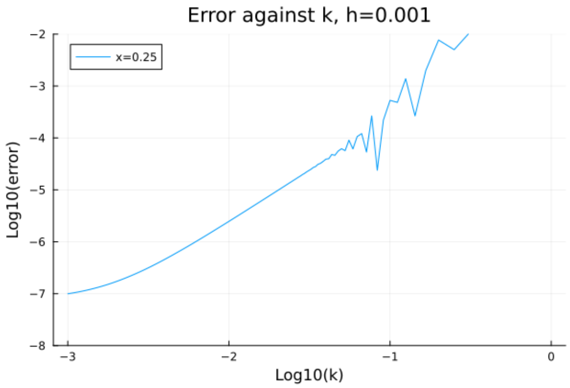
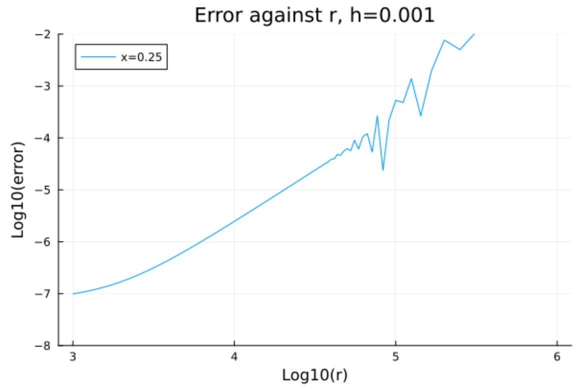


Figure 4: Contour of the solution with the Semi-explicit Crank-Nicholson method on a 101×2001 grid.

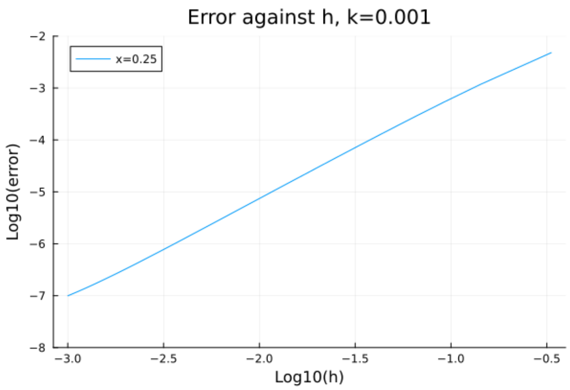
1.7 7



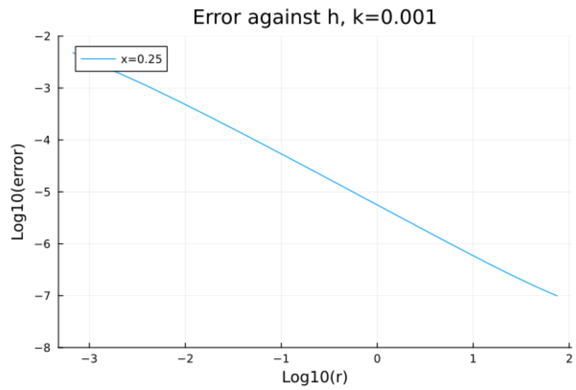
(a) Error with h fixed and k varying



(b) Error with h fixed and r varying



(c) Error with k fixed and h varying



(d) Error with k fixed and r varying

Figure 5: Investigation of relative error with varying h, k and r, at point $x = 0.25$ (Blue).

The figures in Figure 5 above were done similarly to before, fixing h, k, r whilst varying another parameter. The main differences to note here are

- The gradient of all lines present is 2, which reflects the truncation error being of order $O(h^2, k^2)$ rather than $O(h^2, k)$ previously. The change can be seen in (a)
- Since the scheme is unconditionally stable, the scheme can have very large values of r and still be stable (b) (d). There is no transition point anymore.
- In general, we do not need k to be so small anymore to achieve sufficient accuracy. Here, $k = 10^{-3}$ was used in (c) and (d) to achieve 7 digits, whilst previously we needed $k < 10^{-6}$. This is a consequence of the improved truncation error from $O(k)$ to $O(k^2)$.

Hence, the better technique is the semi-explicit method Crank-Nicholson method, as we can achieve similar accuracy with higher values of k in particular. In addition, we no longer need to worry about stability and can choose a much smaller grid size. This greatly outweighs the cost to solve a tridiagonal system many times in terms of computational time.

2 B

2.1 1

The solution to the PDE is approximated by U_n^j on the grid (x_n, t^j) with spacings h and k respectively. To find the order of the truncation error, we first recall the results derived from Taylor series of partial derivatives.

$$\frac{u_n^{j+1} - u_n^{j-1}}{2k} = \frac{\partial u_n^j}{\partial t} + \frac{1}{6}k^2 \frac{\partial^3 u_n^j}{\partial^3 x} + O(k^4) \tag{2.1}$$

$$\frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} = \frac{\partial^2 u_n^j}{\partial^2 x} + \frac{1}{12}h^2 \frac{\partial^4 u_n^j}{\partial^4 x} + O(h^4) \tag{2.2}$$

By setting the partial derivatives equal according to the PDE, we get

$$\frac{u_n^{j+1} - u_n^{j-1}}{2k} = \frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} + R_n^j \tag{2.3}$$

where the truncation error R_n^j is

$$R_n^j = \frac{1}{12}h^2 \frac{\partial^4 u_n^j}{\partial^4 x} + O(h^4) - \frac{1}{6}k^2 \frac{\partial^3 u_n^j}{\partial^3 x} + O(k^4) \tag{2.4}$$

Thus, the order of the trunctation error is $O(h^2, k^2)$. We now use the Fourier method to investigate the stability. Denote the error to be $z_n^j = u_n^j - U_n^j$.

Suppose that at $t = 0$, there is a small error in the numerical and analytic solution $z_n^0 = \varepsilon e^{inph}$, where p is a spatial wavenumber. We only consider the effect of a small complex exponential perturbation, since we can reconstruct any other initial data pertubation using fourier series.

Then after using Equation (2.3) and the numerical scheme (by subtracting one from another), the error z_n^j satisfies the equation

$$\frac{z_n^{j+1} - z_n^{j-1}}{2k} = \frac{z_{n+1}^j - 2z_n^j + z_{n-1}^j}{h^2} + R_n^j \tag{2.5}$$

resulting in the equation for z_n^{j+1}, where we neglected the trunctation error term and used $r = \frac{k}{h^2}$

$$z_n^{j+1} = z_n^{j-1} + 2r(z_{n+1}^j - 2z_n^j + z_{n-1}^j) \tag{2.6}$$

Now suppose that the solution to the recursive formula above is seperable *i.e.* $z_n^j = \varepsilon \xi_j e^{inph}$ for some sequence ξ_j with $\xi_0 = 1$. Hence we derive a recursion relation below.

$$\varepsilon \xi_{j+1} e^{inph} = \varepsilon \xi_{j-1} e^{inph} + 2r(\varepsilon \xi_j e^{i(n+1)ph} - 2\varepsilon \xi_j e^{inph} + \varepsilon \xi_j e^{i(n-1)ph}) \tag{2.7}$$

$$\xi_{j+1} = \xi_{j-1} + 2r(\xi_j e^{iph} - 2\xi_j + \xi_j e^{-iph}) \tag{2.8}$$

$$\xi_{j+1} = \xi_{j-1} + 4r(\cos(ph) - 1)\xi_j \tag{2.9}$$

$$\xi_{j+1} = \xi_{j-1} - 8r \sin^2\left(\frac{ph}{2}\right) \xi_j \tag{2.10}$$

To solve this difference equation, we try the ansatz $\xi_j = \lambda^j$. Upon substitution, we have

$$\lambda^{j+1} = \lambda^{j-1} - 8r \sin^2\left(\frac{ph}{2}\right) \lambda^j \tag{2.11}$$

from which the characteristic equation has solutions

$$\lambda_1 = -4r \sin^2\left(\frac{ph}{2}\right) + \sqrt{16r^2 \sin^4\left(\frac{ph}{2}\right) + 1} \tag{2.12}$$

$$\lambda_2 = -4r \sin^2\left(\frac{ph}{2}\right) - \sqrt{16r^2 \sin^4\left(\frac{ph}{2}\right) + 1} \tag{2.13}$$

and general solution $A\lambda_1^j + B\lambda_2^j$. In order for the errors to not grow, we need both $|\lambda_1| \le 1$ and $|\lambda_2| \le 1$. If $ph = \pi$, we have

$$|\lambda_2| = 4r + \sqrt{16r^2 + 1} > 1 \tag{2.14}$$

Hence, for any value of $r > 0$, the errors grow and the scheme is not stable.

2.2 2

We need the following finite difference formulas derived from Taylor series

$$\frac{u_n^{j+1} - u_n^{j-1}}{2k} = \frac{\partial u_n^j}{\partial t} + \frac{1}{6}k^2\frac{\partial^3 u_n^j}{\partial^3 x} + O(k^4) \tag{2.15}$$
$$\frac{u_{n+1}^j - 2u_n^j + u_{n-1}^j}{h^2} = \frac{\partial^2 u_n^j}{\partial^2 x} + \frac{1}{12}h^2\frac{\partial^4 u_n^j}{\partial^4 x} + O(h^4) \tag{2.16}$$
$$\frac{u_n^{j+1} - 2u_n^j + u_n^{j-1}}{k^2} = \frac{\partial^2 u_n^j}{\partial^2 t} + \frac{1}{12}k^2\frac{\partial^4 u_n^j}{\partial^4 t} + O(k^4) \tag{2.17}$$

By multiplying the third formula by $\frac{k^2}{h^2}$ and subtracting it from the second, we have

$$\frac{u_{n+1}^j - u_n^{j+1} - u_n^{j-1} + u_{n-1}^j}{h^2} = \frac{\partial^2 u_n^j}{\partial^2 x} + \frac{1}{12}h^2\frac{\partial^4 u_n^j}{\partial^4 x} + O(h^4) - \frac{k^2}{h^2}\left(\frac{\partial^2 u_n^j}{\partial^2 t} - \frac{1}{12}k^2\frac{\partial^4 u_n^j}{\partial^4 t} + O(k^4)\right) \tag{2.18}$$

Equating partial derivatives according to the PDE yields

$$\frac{u_{n+1}^j - u_n^{j+1} - u_n^{j-1} + u_{n-1}^j}{h^2} = \frac{u_n^{j+1} - u_n^{j-1}}{2k} + R_n^j \tag{2.19}$$

where we denote the truncation error as R_n^j, which is equal to

$$R_n^j = -\frac{1}{6}k^2\frac{\partial^3 u_n^j}{\partial^3 x} + \frac{1}{12}h^2\frac{\partial^4 u_n^j}{\partial^4 x} + O(k^4, h^4) - \frac{k^2}{h^2}\left(\frac{\partial^2 u_n^j}{\partial^2 t} - \frac{1}{12}k^2\frac{\partial^4 u_n^j}{\partial^4 t} + O(k^4)\right) \tag{2.20}$$

From this we see that in order for R_n^j to go to 0 as $h \to 0$ and $k \to 0$, we also need $\frac{k}{h}$ to go to 0, or equivalently $k = o(h)$.

2.3 3

The basis we will use in the application of the Fourier method is $e^{ilp_xh_x}e^{imp_yh_y}e^{inp_zh_z}$ where p_x, p_y, p_z are wavenumbers in each of the respective directions. As such, we will assume a small exponential perturbation at time $t = 0$ with $z_{lmn}^0 = \varepsilon e^{ilp_xh_x}e^{imp_yh_y}e^{inp_zh_z}$, and assume seperability of the solution *i.e.* $z_{lmn}^j = \xi_j z_{lmn}^0$ for some sequence ξ_j with $\xi_0 = 1$.

First, we will calculate the action of the second order central difference operator on a single term.

$$\delta_x^2 z_{lmn}^j = z_{l+1mn}^j - 2z_{lmn}^j + z_{l-1mn}^j \tag{2.21}$$
$$= \varepsilon\xi_j e^{ilp_xh_x}e^{imp_yh_y}e^{inp_zh_z}(e^{ip_xh_x} - 2 + e^{-ip_xh_x}) \tag{2.22}$$
$$= \xi_j z_{lmn}^0(2\cos(p_xh_x) - 2) \tag{2.23}$$

A similar calculation can be done for δ_y^2, δ_z^2 and also with z_{lmn}^{j+1} with just an exchange of indices.

Thus, since the errors also follow the same recursion relation as the scheme up to ignoring truncation errors, we have

$$z_{lmn}^{j+1} - z_{lmn}^j = k\left[\frac{1}{h_x^2}\delta_x^2 + \frac{1}{h_y^2}\delta_y^2 + \frac{1}{h_z^2}\delta_z^2\right]\left(\theta z_{lmn}^{j+1} + (1-\theta)z_{lmn}^j\right) \tag{2.24}$$

$$\xi_{j+1} z^0_{lmn} - \xi_j z^0_{lmn} = k z^0_{lmn} \left(\theta \xi_{j+1} + (1-\theta)\xi_j\right) \left(\frac{2\cos(p_x h_x) - 2}{h_x^2} + \frac{2\cos(p_y h_y) - 2}{h_y^2} + \frac{2\cos(p_z h_z) - 2}{h_z^2} \right) \tag{2.25}$$

$$\xi_{j+1} - \xi_j = k \left(\theta \xi_{j+1} + (1-\theta)\xi_j\right) A_{xyz} \tag{2.26}$$

where we defined

$$A_{xyz} = A(p_x, h_x, p_y, h_y, p_z, h_z) = \left(\frac{2\cos(p_x h_x) - 2}{h_x^2} + \frac{2\cos(p_y h_y) - 2}{h_y^2} + \frac{2\cos(p_z h_z) - 2}{h_z^2} \right) \tag{2.27}$$

We substitute the ansatz $\xi_j = \lambda^j$ to the linear difference equation.

$$\lambda^{j+1} - \lambda^j = k \left(\theta \lambda^{j+1} + (1-\theta)\lambda^j\right) A_{xyz} \tag{2.28}$$

$$\lambda - 1 = k \left(\theta \lambda + (1-\theta)\right) A_{xyz} \tag{2.29}$$

$$\lambda = \frac{1 + k(1-\theta)A_{xyz}}{1 - k\theta A_{xyz}} = 1 + \frac{kA_{xyz}}{1 - k\theta A_{xyz}} \tag{2.30}$$

We require $|\lambda| \leq 1$ for stability. This is equivalent to the condition that

$$-2 \leq \frac{kA_{xyz}}{1 - k\theta A_{xyz}} \leq 0 \tag{2.31}$$

Note that we have the following bounds on A_{xyz}:

$$-4\left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2}\right) \leq A_{xyz} \leq 0 \tag{2.32}$$

Therefore, continuing on from (2.31), since $1 - k\theta A_{xyz}$ is always positive and non-zero, we have

$$-2(1 - k\theta A_{xyz}) \leq kA_{xyz} \leq 0 \tag{2.33}$$

The second inequality always holds, so we drop it here.

$$-2 + 2k\theta A_{xyz} \leq kA_{xyz} \tag{2.34}$$

$$-2 \leq kA_{xyz}(1 - 2\theta) \tag{2.35}$$

If $\theta \in [\frac{1}{2}, 1]$, then the RHS is always positive (since $A_{xyz} \leq 0$) and the inequality always holds. Hence for these values of θ, the scheme is unconditionally stable. If $\theta \in [0, \frac{1}{2})$, then for stability, we need

$$\frac{2}{1 - 2\theta} \geq -kA_{xyz} \tag{2.36}$$

Since the inequality must hold for all values of A_{xyz}, in particular for the worst case $A_{xyz} = -4\left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2}\right)$ when $p_x h_x = p_y h_y = p_z h_z = \pi$, we have

$$\frac{2}{1 - 2\theta} \geq 4k\left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2}\right) \tag{2.37}$$

which can be rearranged into the result

$$k\left(\frac{1}{h_x^2} + \frac{1}{h_y^2} + \frac{1}{h_z^2}\right) \leq \frac{1}{2(1 - 2\theta)} \tag{2.38}$$