Numerical Solution of Differential Equations I: Problem Sheet 5

1. Suppose that we have discrete data $\{U_j\}$ defined on an infinite grid $x_j = jh$, $j = 0, \pm 1, \pm 2, \ldots$. Let δ and μ be the discrete differentiation and smoothing operators defined by

$$(\delta U)_j = (U_{j+1} - U_{j-1})/(2h)\,, \qquad (\mu U)_j = (U_{j+1} + U_{j-1})/2\,.$$

   a. Determine the functions δU, δV, μU, μV for $U = (\ldots, 1, -1, 1, -1, 1, -1, 1, \ldots)$ and $V = (\ldots, 1, 0, -1, 0, 1, 0, -1, 0, \ldots)$.

   b. Determine what effect δ and μ have on the function U defined by $U_j = \mathrm{e}^{\imath k x_j}$, $j = 0, \pm 1, \pm 2, \ldots$, where k is a real constant (the wave number).

   c. The semi-discrete Fourier transform of a function U defined on the infinite grid $x_j = jh$, $j = 0, \pm 1, \pm 2, \ldots$, is the function $k \mapsto \hat{U}(k)$, $k \in [-\pi/h, \pi/h]$, defined by

$$\hat{U}(k) = h \sum_{j=-\infty}^{\infty} \mathrm{e}^{-\imath k x_j} U_j\,.$$

   [The reason for the restriction on k is that the wave numbers $|k| > \pi/h$ are not resolvable on a grid of spacing h; this is the phenomenon of *aliasing*.]

   Show that the inverse of the semi-discrete Fourier transform is given by the formula

$$U_j = \frac{1}{2\pi} \int_{-\pi/h}^{\pi/h} \mathrm{e}^{\imath k j h} \hat{U}(k)\, \mathrm{d}k\,.$$

   Describe the relationship between $\hat{U}(k)$, and $\widehat{\delta U}(k)$ and $\widehat{\mu U}(k)$.

   The ratios $\widehat{\delta U}/\hat{U}$ and $\widehat{\mu U}/\hat{U}$ are referred to as *Fourier multipliers*. Sketch the graphs of these Fourier multipliers as functions of $k \in [-\pi/h, \pi/h]$.

   One would think that applying μ repeatedly to U should lead to a function that is much smoother than U. Explain this effect by considering a sketch of the multiplier function $\widehat{\mu^m U}/\hat{U}$ for $m \gg 1$. Your analysis should reveal that taking successive powers of μ is not a perfect smoothing procedure. Explain.

2. The $\ell_2(-\infty, \infty)$ norm of U and the $L_2(-\pi/h, \pi/h)$ norm of $\hat{U}$ are defined, respectively, by

$$\|U\|_{\ell_2} = \left(h \sum_{j=-\infty}^{\infty} |U_j|^2 \right)^{1/2}, \qquad \|\hat{U}\|_{L_2} = \left(\int_{-\pi/h}^{\pi/h} |\hat{U}(k)|^2\, \mathrm{d}k \right)^{1/2}.$$

   Prove *Parseval's identity*:

$$\|U\|_{\ell_2} = \frac{1}{\sqrt{2\pi}} \|\hat{U}\|_{L_2}\,.$$

3. Consider the system of linear equations

$$-a_j U_{j-1} + b_j U_j - c_j U_{j+1} = d_j\,, \qquad j = 1, \ldots, J-1\,,$$

   with

$$U_0 = 0\,, \qquad U_J = 0\,,$$

   where $a_j > 0$, $b_j > 0$, $c_j > 0$ and $b_j > a_j + c_j$ for all j.

a) Show that

$$U_j = e_j U_{j+1} + f_j\,, \qquad j = J-1, J-2, \ldots, 1\,, \tag{1}$$

where

$$e_j = \frac{c_j}{b_j - a_j e_{j-1}}\,, \qquad f_j = \frac{d_j + a_j f_{j-1}}{b_j - a_j e_{j-1}}\,, \qquad j = 1, 2, \ldots, J-1\,, \tag{2}$$

with $e_0 = 0$ and $f_0 = 0$. This method for the solution of the linear system of equations (1), (2) is called the *Thomas algorithm.*

b) Show by induction that $0 < e_j < 1$ for $j = 1, 2, \ldots, J-1$. Show further that the conditions

$$b_j > 0\,, \quad b_j \geq |a_j| + |c_j|\,, \qquad j = 1, 2, \ldots, J-1\,,$$

are sufficient to ensure that $|e_j| \leq 1$ for $j = 1, 2, \ldots, J-1$. What do you think the practical significance of the last inequality is regarding the sensitivity of the algorithm to rounding errors.

c) Use matlab to do the following:

(i) Generate any non-zero column vector z with N rows.

(ii) Generate a $N \times N$ tri-diagonal matrix A with value 2 on the diagonal and -1 on the sub- and super-diagonals. Adjust the first and last row to mimic a Dirichlet boundary condition (so for example, $A(1, 2) = 0$).

(iii) Generate a sparse version S of this matrix by `S=sparse(A);`

(iv) Generate a $N \times 3$ matrix B with the vector a in the first column, b in the second column and c in the third column (imagine the tri-diagonal matrix with the diagonal made vertical in the second column).

(v) Use `tic` and `toc` to determine the time taken to calculate

1 `y=A\z ;`

2 `y=S\z ;`

3 Implement the Thomas algorithm in conjunction with the matrix B to determine `y`. (needs a little programming!)

Check that your solutions are working for a small value, for example, $N = 5$. Then calculate times for $N = 10,\ 50,\ 100,\ 250,\ 500,\ 1000$ and plot $\log_{10}$ of the time versus N. Note that times will depend on speed of your computer so only relative times are important. Hence explain why using the full matrix is impractical for large N.

4. Consider the simplest finite difference approximation of the heat equation $u_t = u_{xx}$, given by

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{h^2}\,, \qquad j = \ldots, -2, -1, 0, 1, 2, \ldots\,; \quad n = 0, 1, 2, \ldots\,.$$

What would the analogous difference approximation be based on values of U at just every other point in the x direction, i.e., U_{j+2}^n, U_j^n and U_{j-2}^n? Now suppose that you create a new difference approximation from these two schemes by adding 1/2 of the first difference approximation to 1/2 of the second difference approximation. Using Fourier analysis, explore how large Δt can be in relation to h if this last scheme is to be stable in the $\ell_2(-\infty, \infty)$ norm.

5. (Finals 2010 - a more complex version of the previous question)

Suppose that $h > 0$ is a fixed mesh spacing and let $\mathbb{Z}$ denote the set of all integers.

(a) Let U be a real-valued function, defined on the mesh $\{x_r := rh \ : \ r \in \mathbb{Z}\}$, such that the ℓ^2 norm of U is finite, that is:

$$||U||_{\ell^2} = \left(h \sum_{r=-\infty}^{\infty} |U_r|^2 \right)^{1/2} < \infty.$$

Define the *semi-discrete Fourier transform* $\hat{U}$ of U. Show that Parseval's identity holds, that is,

$$||U||_{\ell^2}^2 = \frac{1}{2\pi} ||\hat{U}||_{\mathrm{L}^2}^2,$$

where

$$||\hat{U}||_{\mathrm{L}^2} = \left(\int_{-\pi/2}^{\pi/2} |\hat{U}(k)|^2 \mathrm{d}k \right)^{1/2}.$$

(b) Consider the initial value problem

$$u_t = \kappa u_{xx}, \quad x \in (-\infty, \infty) \ \ t \in (0, T];$$

$$u(x, 0) = u_0(x), \quad x \in (-\infty, \infty),$$

where κ is a positive real number and u_0 a real-valued function, defined and continuous on $(-\infty, \infty)$ and identically zero outside of a certain bounded closed interval of $\mathbb{R}$.

Let

$$\mathcal{M} := \{(x_r, t_n) \ : \ r \in \mathbb{Z}, n = 0, 1, \ldots, M\},$$

where $x_r = rh$ and $t_n = n\Delta t$ with $\Delta t = T/M$, $M \geq 2$ and $T > 0$. The following finite difference scheme is proposed for the numerical solution of the initial-value problem on the mesh $\mathcal{M}$:

$$\frac{U_r^{n+1} - U_r^n}{\Delta t} = \theta\kappa \frac{U_{r+1}^{n+1} - 2U_r^{n+1} + U_{r-1}^{n+1}}{h^2} + (1-\theta)\kappa \frac{U_{r+2}^n - 2U_r^n + U_{r-2}^n}{(2h)^2}$$

for $r \in \mathbb{Z}$ and $n = 0, 1, \ldots, M-1$ with $U_r^0 = u_0(x_r)$ for $r \in \mathbb{Z}$.

Show, using Parseval's Identity, that

$$||U^{n+1}||_{\ell^2} \leq ||U^n||_{\ell^2}, \quad n = 0, 1, \ldots, M-1,$$

provided that either (i) $\theta \in [0, \frac{1}{2})$ and $\mu(1-2\theta)^2 \leq 2(1-\theta)$ where $\mu = \kappa\Delta t/h^2$, or (ii) $\theta \in [\frac{1}{2}, 1]$,

Deduce that the scheme is conditionally stable in the ℓ^2 norm when $\theta \in [0, \frac{1}{2})$, and unconditionally stable in the ℓ^2 norm when $\theta \in [\frac{1}{2}, 1]$.