APM 522

Problem Set 1

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1 Problem 1

Largest possible number:

$$2^{127} = 1.70 \times 10^{38} \tag{1.1}$$

Smallest possible number:

$$\frac{1}{2} \cdot 2^{-128} = 2^{-129} = 1.47 \times 10^{-39} \tag{1.2}$$

Machine Epsilon:

$$\epsilon_M = \frac{1}{2} \cdot 2^{-55} = 2^{-56} = 1.39 \times 10^{-17} \tag{1.3}$$

2 Problem 2

2.1 Part a

Starting with the three-point central difference formula for $\partial f/\partial x$,

$$\frac{\partial f}{\partial x} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} \tag{2.1}$$

Taking a Taylor Series expansion about i gives,

$$\begin{aligned} \frac{\partial f}{\partial x} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} =& \frac{1}{2\Delta x}\Bigg[\left(f_i + \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' + \frac{\Delta x^3}{6} f_i''' + \dots\right) \\ & - \left(f_i - \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' - \frac{\Delta x^3}{6} f_i''' \pm \dots\right)\Bigg] \end{aligned} \tag{2.2}$$

Next combining like terms gives,

$$\frac{\partial f}{\partial x} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} = \frac{1}{2\Delta x}\left(2\Delta x f_i' + \frac{1}{3}\Delta x^3 f_i''' + \dots\right) \tag{2.3}$$

thus

$$\frac{\partial f}{\partial x} \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x} = f_i' + \frac{1}{6}\Delta x^2 f_i''' + \dots \tag{2.4}$$

Clearly from Eqn. (2.5) the finite difference scheme is of $O(2)$.

2.2 Part b

Starting with the three-point central difference formula for $\partial^2 f/\partial x^2$,

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} \tag{2.5}$$

Taking a Taylor Series expansion about i gives,

$$\begin{aligned} &\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} = \\ &\frac{1}{\Delta x^2}\Bigg[\left(f_i + \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' + \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i^{(4)} + \dots\right) \\ &- 2f_i + \left(f_i - \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' - \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i^{(4)} \pm \dots\right)\Bigg] \end{aligned} \tag{2.6}$$

Next combining like terms gives,

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} = \frac{1}{\Delta x^2}\left(\Delta x^2 f_i'' + \frac{1}{12}\Delta x^4 f_i^{(4)} + \ldots\right) \tag{2.7}$$

thus

$$\frac{\partial^2 f}{\partial x^2} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} = f_i'' + \frac{1}{12}\Delta x^2 f_i^{(4)} + \ldots \tag{2.8}$$

Clearly from Eqn. (2.8) the finite difference scheme is of $O\left(2\right)$.

2.3 Part c

Starting with the one-sided finite difference scheme, namely

$$\frac{\mathrm{d}u}{\mathrm{d}t} \approx \frac{u^{n+1} - u^n}{\Delta t} \tag{2.9}$$

Taking a Taylor Series expansion about n gives,

$$\frac{\mathrm{d}u}{\mathrm{d}t} \approx \frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{\Delta t^t}\left[\left(u^n + \Delta t \dot{u}^n + \frac{1}{2}\Delta t^2 \ddot{u}^n + \ldots\right) - u^n\right] \tag{2.10}$$

where $\dot{(\ )} \equiv \frac{\mathrm{d}}{\mathrm{d}t}\left(\ \right)$. Combining like terms gives,

$$\frac{\mathrm{d}u}{\mathrm{d}t} \approx \frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{\Delta t}\left(\Delta t \dot{u}^n + \frac{1}{2}\Delta t^2 \ddot{u}^n + \ldots\right) \tag{2.11}$$

thus

$$\frac{\mathrm{d}u}{\mathrm{d}t} \approx \frac{u^{n+1} - u^n}{\Delta t} = \dot{u}^n + \frac{1}{2}\Delta t \ddot{u}^n + \ldots \tag{2.12}$$

From Eqn. (2.11) the finite difference scheme is clearly of $O\left(1\right)$.

3 Problem 3

Start by taking the TS of each of the four stencil points about j,

$$f_{j+2} = f_j + 2\Delta x f_j' + 2\Delta x^2 f_j'' + \frac{4}{3}\Delta x^3 f_j''' + \frac{2}{3}\Delta x^4 f_j^{(4)} + \frac{4}{15}\Delta x^5 f_j^{(5)} + \dots \tag{3.1a}$$

$$f_{j+1} = f_j + \Delta x f_j' + \frac{1}{2}\Delta x^2 f_j'' + \frac{1}{6}\Delta x^3 f_j''' + \frac{1}{24}\Delta x^4 f_j^{(4)} + \frac{1}{120}\Delta x^5 f_j^{(5)} + \dots \tag{3.1b}$$

$$f_{j-1} = f_j - \Delta x f_j' + \frac{1}{2}\Delta x^2 f_j'' - \frac{1}{6}\Delta x^3 f_j''' + \frac{1}{24}\Delta x^4 f_j^{(4)} - \frac{1}{120}\Delta x^5 f_j^{(5)} \pm \dots \tag{3.1c}$$

$$f_{j-2} = f_j - 2\Delta x f_j' + 2\Delta x^2 f_j'' - \frac{4}{3}\Delta x^3 f_j''' + \frac{2}{3}\Delta x^4 f_j^{(4)} - \frac{4}{15}\Delta x^5 f_j^{(5)} \pm \dots \tag{3.1d}$$

Substituting Eqns. (3.1a-3.1d) into the finite difference approximation gives,

$$\begin{aligned}
&\left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_j \approx \frac{1}{\Delta x}\left[-\frac{1}{12}f_{j+2} + \frac{2}{3}f_{j+1} - \frac{2}{3}f_{j-1} + \frac{1}{12}f_{j-2}\right] = \\
&\frac{1}{\Delta x}\Bigg[-\frac{1}{12}\left(f_j + 2\Delta x f_j' + 2\Delta x^2 f_j'' + \frac{4}{3}\Delta x^3 f_j''' + \frac{2}{3}\Delta x^4 f_j^{(4)} + \frac{4}{15}\Delta x^5 f_j^{(5)} + \dots\right) \\
&+\frac{2}{3}\left(f_j + \Delta x f_j' + \frac{1}{2}\Delta x^2 f_j'' + \frac{1}{6}\Delta x^3 f_j''' + \frac{1}{24}\Delta x^4 f_j^{(4)} + \frac{1}{120}\Delta x^5 f_j^{(5)} + \dots\right) \\
&-\frac{2}{3}\left(f_j - \Delta x f_j' + \frac{1}{2}\Delta x^2 f_j'' - \frac{1}{6}\Delta x^3 f_j''' + \frac{1}{24}\Delta x^4 f_j^{(4)} - \frac{1}{120}\Delta x^5 f_j^{(5)} \pm \dots\right) \\
&+\frac{1}{12}\left(f_j - 2\Delta x f_j' + 2\Delta x^2 f_j'' - \frac{4}{3}\Delta x^3 f_j''' + \frac{2}{3}\Delta x^4 f_j^{(4)} - \frac{4}{15}\Delta x^5 f_j^{(5)} \pm \dots\right)\Bigg]
\end{aligned} \tag{3.2}$$

Combining like terms in Eqn. (3.2) one gets the following,

$$\begin{aligned}
&\left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_j \approx \frac{1}{\Delta x}\left[-\frac{1}{12}f_{j+2} + \frac{2}{3}f_{j+1} - \frac{2}{3}f_{j-1} + \frac{1}{12}f_{j-2}\right] = \\
&\frac{1}{\Delta x}\left(\Delta x f_j' - \frac{1}{30}\Delta x^5 f_j^{(5)} + \dots\right)
\end{aligned} \tag{3.3}$$

thus

$$\left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)_j \approx \frac{1}{\Delta x}\left[-\frac{1}{12}f_{j+2} + \frac{2}{3}f_{j+1} - \frac{2}{3}f_{j-1} + \frac{1}{12}f_{j-2}\right] = f_j' - \frac{1}{30}\Delta x^4 f_j^{(5)} \tag{3.4}$$

Clearly from Eqn. (3.4) the finite difference approximation is of $O(4)$.

4 Problem 4

Start by showing that $K(x,t)$ satisfies the general heat equation which is expressed in index notation below

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x_j}\left(\kappa \frac{\partial u}{\partial x_j}\right) \tag{4.1}$$

which for 1-D and a constant diffusivity coefficient κ Eqn (4.1) reduces to

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} \tag{4.2}$$

Substituting $K(x,t)$

$$\frac{1}{\sqrt{4\pi\kappa t}} \exp\left(-\frac{x^2}{4\kappa t}\right) \tag{4.3}$$

into Eqn. (4.2) gives the following,

$$\frac{\partial K}{\partial t} = \frac{-\exp\left(\frac{x^2}{4\kappa t}\right)\left(2\kappa t - x^2\right)}{8\kappa t^2 \sqrt{\kappa \pi t}} \tag{4.4}$$

$$\frac{\partial K}{\partial x} = \frac{-x \exp\left(\frac{x^2}{4\kappa t}\right)}{4\sqrt{\pi}\left(\kappa t\right)^{3/2}} \tag{4.5}$$

$$\frac{\partial^2 K}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial K}{\partial x}\right) = \exp\left(\frac{x^2}{4\kappa t}\right)\left(\frac{x^2}{8\sqrt{\pi}\left(\kappa t\right)^{5/2}} - \frac{1}{4\sqrt{\pi}\left(\kappa t\right)^{3/2}}\right) \tag{4.6}$$

thus

$$\kappa \frac{\partial^2 K}{\partial x^2} = \frac{-\exp\left(\frac{x^2}{4\kappa t}\right)\left(2\kappa t - x^2\right)}{8\kappa t^2 \sqrt{\kappa \pi t}} = \frac{\partial K}{\partial t} \tag{4.7}$$

Therefore $K(x,t)$ satisfies Eqn. (4.2). Next we show that $u(x,t)$,

$$u(x,t) = \int_{-\infty}^{\infty} K(x-y,t)\, u_0(y)\, dy \tag{4.8}$$

also satisfies the heat the 1-D linear heat equation. We start by substituting in Eqn. (4.8) into each of the two partial derivatives, namely

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} K(x-y,t)\, u_0(y)\, dy \tag{4.9a}$$

$$\kappa \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} K(x-y,t)\, u_0(y)\, dy \tag{4.9b}$$

Next we switch the order of the partial derivative and integration operators giving,

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial t} K(x-y,t)\, u_0(y)\, dy \tag{4.10a}$$

$$\int_{-\infty}^{\infty} \kappa \frac{\partial^2}{\partial x^2} K(x-y,t)\, u_0(y)\, dy \tag{4.10b}$$

Since we are not taking any derivative with respect to y in Eqn. (4.10) we can simply treat it as a constant thus

$$\int_{-\infty}^{\infty} K(x-y,t)_t\, u_0(y)\, dy \tag{4.11a}$$

$$\int_{-\infty}^{\infty} \kappa K(x-y,t)_{xx}\, u_0(y)\, dy \tag{4.11b}$$

Furthermore, it was shown in Eqn. (4.7) that $K(x,t)_y = \kappa K(x,t)_{xx}$ therefore

$$\frac{\partial u(x,t)}{\partial t} = \int_{-\infty}^{\infty} K(x-y,t)_t\, u_0(y)\, dy = \int_{-\infty}^{\infty} \kappa K(x-y,t)_{xx}\, u_0(y)\, dy = \kappa \frac{\partial^2 u(x,t)}{\partial x^2} \tag{4.12}$$

thus

$$\frac{\partial u(x,t)}{\partial t} = \kappa \frac{\partial^2 u(x,t)}{\partial x^2} \tag{4.13}$$

Lastly we show $u(x,t)$ satisfies the initial condition of $u(x,t=0) = u_0(x)$ by taking limit of $u(x,t)$ of $t \to 0$,

$$u(x,t=0) = \lim_{t\to 0} \int_{-\infty}^{\infty} K(x-y,t)\, u_0(y)\, dy \tag{4.14}$$

Recognizing that this gives the (Dirac) delta function which $\int_{-\infty}^{\infty} \delta(x-a)\, f(x) = f(a)$ gives,

$$u(x,t=0) = \lim_{t\to 0} \int_{-\infty}^{\infty} K(x-y,t)\, u_0(y)\, dy = u_0(x) \tag{4.15}$$

Therefore $u(x,t)$ satisfies both the partial differential equation and the initial condition making it a solution to the 1-D linear heat equation.

5 Problem 5

Starting with the Trapezoidal Rule:

$$u_i^{n+1} = u_i^n + \frac{\Delta t}{2\Delta x^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n + u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right) + \Delta t \tau \tag{5.1}$$

Next we expand the right hand about t and the left hand side about i,

$$u_i^{n+1} = u_i^n + \Delta t u_{i,t}^n + \frac{\Delta t^2}{2} u_{i,tt}^n + \frac{\Delta t^3}{6} u_{i,ttt}^n + \dots \tag{5.2a}$$

$$u_{i+1}^n = u_i^n + \Delta x u_{i,x}^n + \frac{\Delta x^2}{2} u_{i,xx}^n + \frac{\Delta x^3}{6} u_{i,xxx}^n + \frac{\Delta x^4}{24} u_{i,xxxx}^n + \dots \tag{5.2b}$$

$$u_{i-1}^n = u_i^n - \Delta x u_{i,x}^n + \frac{\Delta x^2}{2} u_{i,xx}^n - \frac{\Delta x^3}{6} u_{i,xxx}^n + \frac{\Delta x^4}{24} u_{i,xxxx}^n \pm \dots \tag{5.2c}$$

$$u_{i+1}^{n+1} = u_i^{n+1} + \Delta x u_{i,x}^{n+1} + \frac{\Delta x^2}{2} u_{i,xx}^{n+1} + \frac{\Delta x^3}{6} u_{i,xxx}^{n+1} + \frac{\Delta x^4}{24} u_{i,xxxx}^{n+1} + \dots \tag{5.2d}$$

$$u_{i-1}^{n+1} = u_i^{n+1} - \Delta x u_{i,x}^{n+1} + \frac{\Delta x^2}{2} u_{i,xx}^{n+1} - \frac{\Delta x^3}{6} u_{i,xxx}^{n+1} + \frac{\Delta x^4}{24} u_{i,xxxx}^{n+1} \pm \dots \tag{5.2e}$$

Note that the subscript notation contains both the spatial grid point and the partial derivative i.e., $u_{i,t}^n$ means take the partial derivative with respect to t at grid point i and time-step n. Next Eqn. (5.2) is substituted into Eqn. (5.1) and all like terms are combined giving,

$$\begin{aligned} u_i^n + \Delta t u_{i,t}^n + \frac{\Delta t^2}{2} u_{i,tt}^n + \frac{\Delta t^3}{6} u_{i,ttt}^n + \dots = \\ u_i^n + \frac{\Delta t}{2\Delta x^2}\left(\Delta x^2 u_{i,xx}^n + \frac{\Delta x^4}{12} u_{i,xxxx}^n + \Delta x^2 u_{i,xx}^{n+1} + \frac{\Delta x^4}{12} u_{i,xxxx}^{n+1} + \dots\right) + \Delta t \tau \end{aligned} \tag{5.3}$$

Furthermore the terms inside the parentheses of the left hand side can be expressed as the partial derivative terms that appear on the right hand side,

$$u_{i,xx}^n = u_{i,t}^n \tag{5.4a}$$

$$\begin{aligned} u_{i,xx}^{n+1} &= u_{i,xx}^n + \Delta t u_{i,xxt}^n + \frac{\Delta t^2}{2} u_{i,xxtt}^n + \dots \\ &= u_{i,t}^n + \Delta t u_{i,tt}^n + \frac{\Delta t^2}{2} u_{i,ttt}^n + \dots \end{aligned} \tag{5.4b}$$

$$u_{i,xxxx}^{n+1} = u_{i,xxxx}^n + \dots \tag{5.4c}$$

Substituting in Eqn. (5.4) into Eqn. (5.3) gives

$$\begin{aligned} u_i^n + \Delta t u_{i,t}^n + \frac{\Delta t^2}{2} u_{i,tt}^n + \frac{\Delta t^3}{6} u_{i,ttt}^n + \dots = \\ u_i^n + \frac{\Delta t}{2\Delta x^2}\Big(\Delta x^2 u_{i,t}^n + \frac{\Delta x^4}{12} u_{i,xxxx}^n + \Delta x^2 u_{i,t}^n + \\ \Delta x^2 \Delta t u_{i,tt}^n + \frac{\Delta x^2 \Delta t^2}{2} u_{i,ttt}^n + \frac{\Delta x^4}{12} u_{i,xxxx}^n + \dots\Big) + \Delta t \tau \end{aligned} \tag{5.5}$$

Combing like terms produces

$$\begin{aligned} u_i^n + \Delta t u_{i,t}^n + \frac{\Delta t^2}{2} u_{i,tt}^n + \frac{\Delta t^3}{6} u_{i,ttt}^n + \ldots = \\ u_i^n + \Delta t u_{i,t}^n + \frac{\Delta t^2}{2} u_{i,tt}^n + \frac{\Delta t^3}{4} u_{i,ttt}^n + \frac{\Delta x^2}{12} u_{i,xxxx}^n + \ldots + \Delta t \tau \end{aligned} \tag{5.6}$$

Next we can solve for the LTE (Δt^τ) by subtracting the left hand side from the right hand side, namely

$$\tau \Delta t = -\frac{\Delta t^3}{12} u_{i,ttt}^n - \frac{\Delta t \Delta x^2}{12} u_{i,xxxx}^n \tag{5.7}$$

thus

$$\tau = -\frac{\Delta t^2}{12} u_{i,ttt}^n - \frac{\Delta x^2}{12} u_{i,xxxx}^n = c_1 \Delta t^2 + c_2 \Delta x^2 \tag{5.8}$$

Therefore,

$$c_1 = -\frac{1}{12} u_{i,ttt}^n \tag{5.9a}$$

$$c_2 = -\frac{1}{12} u_{i,xxxx}^n \tag{5.9b}$$