Numerical Simulations Homework # 3

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1 Problem 1

1.1 Part a

Our exact function is \widetilde{T} , which has the general Taylor series:

$$\frac{\partial \widetilde{T}}{\partial x} = \widetilde{T}(x_0) + \Delta x \frac{\partial \widetilde{T}}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 \widetilde{T}}{\partial x^2} + \frac{\Delta x^3}{6} \frac{\partial^3 \widetilde{T}}{\partial x^3} + \dots$$

We are approximating this derivative via three pieces: a spatial step "back," the current location, and a spatial step forward:

$$\left[\frac{\partial \widetilde{T}}{\partial x}\right]_{j}^{n} = a\widetilde{T}_{j-1}^{n} + b\widetilde{T}_{j}^{n} + c\widetilde{T}_{j+1}^{n} + O(\Delta x^{m})$$

and either of the two spatial steps can be expressed as Taylor series. The \tilde{T}_{j-1}^n term is with a spatial step of $-\Delta x$, meaning its Taylor series, with a coefficient of a, will alternate sign. Meanwhile, the \tilde{T}_{j+1}^n term is with a spatial step of $+\Delta x$. Our current position, \tilde{T}_j^n , has no associated Δx , giving us only the $b\tilde{T}_j^n$ term. Combine these two series and our $b\tilde{T}_j^n$ term and we have

$$\left[\frac{\partial \widetilde{T}}{\partial x}\right]_{j}^{n} = (a+b+c)\widetilde{T}_{j}^{n} + (-a+c)\Delta x \left[\frac{\partial \widetilde{T}}{\partial x}\right]_{j}^{n} + (a+c)\frac{\Delta x^{2}}{2} \left[\frac{\partial^{2} \widetilde{T}}{\partial x^{2}}\right]_{j}^{n} + (-a+c)\frac{\Delta x^{3}}{6} \left[\frac{\partial^{3} \widetilde{T}}{\partial x^{3}}\right]_{j}^{n} + \dots$$

1.2 Part b

Since we have

$$\left[\frac{\partial \tilde{T}}{\partial x}\right]_{j}^{n} = a\tilde{T}_{j-1}^{n} + b\tilde{T}_{j}^{n} + c\tilde{T}_{j+1}^{n} + O(\Delta x^{m})$$

we know that our coefficients of \widetilde{T}_j^n must vanish, i.e. a+b+c=0. Likewise, we want $(-a+c)\Delta x=1$ to return our first order derivative. Thus, $a=c-1/\Delta x$ and $b=-2c+1/\Delta x$. Note that since a and c depend on $1/\Delta x$, the term we wish to eliminate in our Taylor approximation is the $(a+c)\Delta x^2$ term. Thus, $a=-c=-1/2\Delta x$ and b=0. This gives us a final approximation of

$$\left[\frac{\partial \widetilde{T}}{\partial x}\right]_{i}^{n} = \frac{\widetilde{T}_{j+1}^{n} - \widetilde{T}_{j-1}^{n}}{2\Delta x} + O(\Delta x^{2})$$

1.3 Part c

Working with the second derivative, now we want $(a+c)\Delta x^2/2 = 1$, so $a = -c + 2/\Delta x^2$, and we also know $(-a+c)\Delta x^3/6 = 0$ to zero out what will become our Δx term. So $a = c = 1/\Delta x^2$, and from our first term, a+b+c=0 so $b=-2/\Delta x^2$. Thus we obtain

$$\left[\frac{\partial^2 \widetilde{T}}{\partial x^2}\right]_j^n = \frac{\widetilde{T}_{j+1}^n - 2\widetilde{T}_j^n + \widetilde{T}_{j-1}^n}{\Delta x^2} + O(\Delta x^2)$$

2 Problem 2

2.1 Part a

For $y = \sin \pi x/2$, we are evaluating dy/dx at x = 0.5. Explicitly, $dy/dx = (\pi/2)\cos \pi x/2$.

Three point symmetric error:

$$\frac{dy}{dx} \approx \frac{y_{j+1} - y_{j-1}}{2\Delta x} = \frac{\sin 0.3\pi - \sin 0.2\pi}{2 \times 0.1} \approx 1.10616$$

Our error is $\pi/2\cos\pi x/2$ minus the above, which is -0.0045620. We compare this to

$$\Delta x^2 \frac{f_{xxx}}{6} = (0.1^2) \frac{(-\pi/2)^3 \cos 0.25\pi}{6} \approx -0.0045677$$

which differs by 5 parts in one million.

Forward difference:

$$\frac{dy}{dx} \approx \frac{y_{j+1} - y_j}{\Delta x} = \frac{\sin 0.3\pi - \sin 0.25\pi}{0.1} \approx 1.019102$$

Our error is $\pi/2\cos \pi x/2$ minus the above, which is 0.091618.

We compare this to

$$\Delta x \frac{f_{xx}}{2} = 0.1 \frac{(\pi/2)^2 (-\sin 0.25\pi)}{2} \approx 0.01935900$$

which differs by eight parts in one hundred.

Five point symmetric error:

$$\frac{dy}{dx} \approx \frac{y_{j+2} - 8y_{j+1} + 8y_{j-1} - y_{j-2}}{12\Delta x} \approx 1.1106982$$

Our error is $\pi/2\cos\pi x/2$ minus the above, which is 2.2474×10^{-5} . We compare this to

$$\Delta x^4 \frac{f_{xxxxx}}{30} = 10^{-5} \frac{(\pi/2)^5 (\cos 0.25\pi)}{30} \approx 3.177879 \times 10^{-6}$$

3 Problem 3

3.1 Part a

Our equation is

$$\frac{\partial \widetilde{T}}{\partial t} - \alpha \frac{\partial^2 \widetilde{T}}{\partial x^2} = 0$$

We insert our first and second derivative expanisons from Problem 1 and include only first-order terms. Note we only have a forward step in time, not a centered derivative like in the spatial terms.

$$\frac{\widetilde{T}_j^{n+1} - \widetilde{T}_j^n}{\Delta t} - \alpha \frac{\widetilde{T}_{j+1}^n - 2\widetilde{T}_j^n + \widetilde{T}_{j-1}^n}{\Delta x^2} = 0$$

$$\widetilde{T}_{j}^{n+1} - \widetilde{T}_{j}^{n} = \frac{\alpha \Delta t}{\Delta x^{2}} \left(\widetilde{T}_{j+1}^{n} - 2\widetilde{T}_{j}^{n} + \widetilde{T}_{j-1}^{n} \right)$$

Let $\alpha \Delta t / \Delta x^2 = s$, so we have

$$\widetilde{T}_{j}^{n+1} = \widetilde{T}_{j}^{n} + s \left(\widetilde{T}_{j+1}^{n} - 2\widetilde{T}_{j}^{n} + \widetilde{T}_{j-1}^{n} \right)$$

$$\widetilde{T}_j^{n+1} = s\widetilde{T}_{j+1}^n + (1-2s)\widetilde{T}_j^n + s\widetilde{T}_{j-1}^n$$

3.2 Part c

The five-point symmetric scheme should converge much more rapidly.