Physics 371: Midterm 2

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Problem 1: FFT (25 pts.)

Consider the function $f(x)$ represented on a set of equally spaced grid points $x_i = i$ with $i=0,\ldots,N-1$. For the case $N=27$, derive the fast Fourier transform algorithm. Show that the scaling in this case is $N\log N$.

$\rightarrow f_j$ need $\tilde{f}_k = \sum_{j=0}^{N-1} e^{i\frac{2\pi}{N}jk} f_j$

$j = 9j_9 + 3j_3 + j_1$ $\qquad j_9 = 0, 1, 2$

$k = 9k_9 + 3k_3 + k_1$ $\qquad j_3 = 0, 1, 2$

$\qquad j_1 = 0, 1, 2$

$$\tilde{f}(k_9, k_3, k_1) = \sum_{j_9=0,1,2} \sum_{j_3=0,1,2} \sum_{j_1=0,1,2} e^{i\frac{2\pi}{N}(9j_9+3j_3+j_1)(9k_9+3k_3+k_1)} \times f(j_9, j_3, j_1)$$

$$(9j_9 + 3j_3 + j_1)(9k_9 + 3k_3 + k_1)$$
$$= 81 j_9 k_9 + 27 j_9 k_3 + 9 j_9 k_1$$
$$+ 27 j_3 k_9 + 9 j_3 k_3 + 3 j_3 k_1$$
$$+ 9 j_1 k_9 + 3 j_1 k_3 + j_1 k_1$$

$w = e^{i\frac{2\pi}{N}}$

$N = 27$

$$\tilde{f}(k_9, k_3, k_1) = \sum_{j_9=0}^{2} \sum_{j_3=0}^{2} \sum_{j_1=0}^{2} w^{9j_9k_1 + 9j_3k_3 + 9j_1k_9 + 3j_3k_1 + 3j_1k_3 + j_1k_1} f(j_9, j_3, j_1)$$

define $\tilde{f}_1(k_1, j_3, j_1) = \sum_{j_9=0}^{2} f(j_9, j_3, j_1) w^{9j_9k_1}$

$$\tilde{f}_1(k_1, j_3, j_1) = f(0, j_3, j_1) + f(1, j_3, j_1) w^{9k_1} + f(2, j_3, j_1) w^{18k_1}$$

$$\tilde{f}(k_9, k_3, k_1) = \sum_{j_3=0}^{2} \sum_{j_1=0}^{2} w^{9j_3k_3 + 9j_1k_9 + 3j_3k_1 + 3j_1k_3 + j_1k_1} \times \tilde{f}_1(k_1, j_3, j_1)$$

(con't on worksheet 4)

Problem 2: Diffusion equation (25 pts.)

Consider the diffusion equation in a finite region from 0 to L, given by

$$\frac{\partial}{\partial t}\Psi(x,t) = \kappa \frac{\partial^2}{\partial x^2}\Psi(x,t).$$

and with mixed boundary conditions,

$\frac{\partial}{\partial x}\Psi(0,t) = 0$, and $\Psi(L,t) = 0$.

1. Construct a grid of N points on which the centered derivative approximation for the variable x can be implemented. (5 pts.)
2. Derive the equations for the forward time centered space scheme which solves the diffusion equation in this case. (10 pts.)
3. Given the following information: $N = 4$, $\Psi(0,t) = A$, and $\Psi_3^0 = B$, perform one propagation step analytically. In other words determine Ψ_i^1 for all i ($i = 1, ..., 4$). (10 pts.)

1.) grid:

2.) FTCS: $\psi_i^n = \Psi(\Delta x\, i, \Delta t\, n)$ ($\Psi(x,t)$ is solution)

$$\frac{\partial\Psi}{\partial t} \to \frac{\Psi_i^{n+1} - \Psi_i^n}{\Delta t}$$

$$\frac{\partial^2\Psi}{\partial x^2} \to \frac{\Psi_{i+1}^n + \Psi_{i-1}^n - 2\Psi_i^n}{\Delta x^2}$$

$$\to \Psi_i^{n+1} = \Psi_i^n + \frac{\kappa \Delta t}{\Delta x^2}\left[\Psi_{i+1}^n + \Psi_{i-1}^n - 2\Psi_i^n\right]$$

at boundaries: $i = N \Rightarrow \Psi_i^n = 0$ if $i = N$

($x=L$) $\Psi_{N-1}^{n+1} = \Psi_{N-1}^n + \frac{\kappa \Delta t}{\Delta x^2}\left[\Psi_{N-2}^n - 2\Psi_{N-1}^n\right]$

($x=0$) $\Psi_1^n = \Psi_2^n$ $\longrightarrow$

$\Psi_1^{n+1} = \Psi_2^{n+1} = \Psi_2^n + \frac{\kappa \Delta t}{\Delta x^2}\left[\Psi_3^n - \Psi_2^n\right]$

$\Psi_3^{n+1} = \Psi_3^n + \frac{\kappa \Delta t}{\Delta x^2}\left[\Psi_4^n + \Psi_2^n - 2\Psi_3^n\right]$

$\vdots$

continue on worksheet 2

Problem 3: Galerkin method (25 pts.)

Consider the ordinary differential equation $f' = f$ on the interval $0 \leq t \leq 1$, with $f(0) = 1$. We construct an approximate solution of the form $f_x(t) = a_0 + a_1 t + a_2 t^2$. Find the coefficients a_0, a_1, a_2. (Notice that the basis functions are not orthogonal, but that is not a necessary condition.)

$f_x(t) = a_0 + a_1 t + a_2 t^2$

$f_x(0) = a_0 = 1 \quad \Rightarrow \boxed{a_0 = 1}$

$f_x'(t) = a_1 + 2a_2 t$

residual: $[a_1 + 2a_2 t - 1 - a_1 t - a_2 t^2] = 0$

$\cancel{a_1(1-t)}$

$a_1 - 1 + (2a_2 - a_1)t - a_2 t^2 = 0$

functions: t, t^2 $\quad \int_0^1 dt = 1 \quad \int_0^1 t\,dt = \frac{1}{2} \quad \int_0^1 t^4 dt = \frac{1}{5}$

$\int_0^1 t^2 dt = \frac{1}{3} \quad \int_0^1 t^3 dt = \frac{1}{4}$

$\frac{(a_1 - 1)}{2} + \frac{(2a_2 - a_1)}{3} - \frac{a_2}{4} = 0$

$\frac{(a_1 - 1)}{3} + \frac{(2a_2 - a_1)}{4} - \frac{a_2}{5} = 0$

$\frac{1}{6} a_1 + \frac{5}{12} a_2 = \frac{1}{2} \Rightarrow a_1 + \frac{5}{2} a_2 = 3$

$\frac{1}{12} a_1 + \frac{3}{10} a_2 = \frac{1}{3} \rightarrow a_1 + \frac{18}{5} a_2 = 4$

$\left(\frac{5}{2} - \frac{18}{5}\right) = \frac{25 - 36}{10} = -\frac{11}{10}$

$\boxed{a_2 = \frac{10}{11}}$

$a_1 = 4 - \frac{18}{5} \cdot \frac{10}{11} = 4 - \frac{36}{11} = \frac{44 - 36}{11} = \frac{8}{11}$

$\boxed{a_1 = \frac{8}{11}}$

Problem 4: Implicit method for the diffusion equation (25 pts.)

Derive an implicit method to solve the diffusion equation with periodic boundary conditions (15 pts.). Perform a stability analysis on the method (10 pts.).

$$\vec{\Psi}_f^{n+1} = \vec{\Psi}_f^n + \hat{M}\vec{\Psi}^n \qquad \hat{M} = \begin{bmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \\ 0 & & 1 & -2 \end{bmatrix} \cdot \frac{\kappa \Delta t}{\Delta x^2}$$

$$\vec{\Psi}^{n+1} = \vec{\Psi}^n + \hat{M}\left(\frac{\vec{\Psi}^{n+1} + \vec{\Psi}^n}{2}\right)$$

$$\left(\hat{I} - \frac{\hat{M}}{2}\right)\vec{\Psi}^{n+1} = \left(\hat{I} + \frac{\hat{M}}{2}\right)\vec{\Psi}^n$$

$$\vec{\Psi}^{n+1} = \left(\hat{I} - \frac{\hat{M}}{2}\right)^{-1}\left(\hat{I} + \frac{\hat{M}}{2}\right)\vec{\Psi}^n$$

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stability analysis

1.) ~~dta.~~ determine largest eigenvalue of matrix $\left(\hat{I} - \frac{\hat{M}}{2}\right)^{-1}\left(\hat{I} + \frac{\hat{M}}{2}\right)$

by operating on an arbitrary vector a large number of times

$$\Rightarrow \hat{A} = \left(\hat{I} - \frac{\hat{M}}{2}\right)^{-1}\left(\hat{I} + \frac{\hat{M}}{2}\right)$$

$$\hat{A}^n \vec{\Psi}^0 = \hat{A}^n \sum_i a_i |i\rangle = \sum_i \boxed{\lambda_i^n} a_i |i\rangle$$

largest term will dominate for many $(n \to \infty)$

2.) Fourier method

$$\Psi_i^{n+1} = \Psi_i^n + \frac{\kappa \Delta t}{2\Delta x^2}\left(\Psi_{i+1}^{n+1} + \Psi_{i-1}^{n+1} - 2\Psi_i^{n+1}\right) + \frac{\kappa \Delta t}{2\Delta x^2}\left(\Psi_{i+1}^n + \Psi_{i-1}^n - 2\Psi_i^n\right)$$

(con't on worksheet 3)

Worksheet 1:

define: $\tilde{f}_2(k_1, k_3, j_1) = \sum_{j_3=0}^{2} w^{9 j_3 k_3 + 3 j_3 k_1} \tilde{f}_1(k_1, j_3, j_1)$

$$= \tilde{f}_1(k_1, 0, j_1) + w^{9k_3 + 3k_1} \tilde{f}(k_1, 1, j_1) + w^{18k_3 + 6k_1} \tilde{f}(k_1, 2, j_1)$$

$$\tilde{f}_3(k_1, k_3, k_9) = \sum_{j_1=0}^{2} w^{9 j_1 k_9 + 3 j_1 k_3 + j_1 k_1} \tilde{f}_2(k_1, k_3, j_1)$$

$$= \tilde{f}_2(k_1, k_3, 0) + w^{9k_9 + 3k_3 + k_1} \tilde{f}(k_1, k_3, 1) + w^{18k_9 + 6k_3 + 2k_1} \tilde{f}(k_1, k_3, 2)$$

$\tilde{f}_3(k_1, k_3, k_9) \rightarrow$ FT result wanted

how many operations?

<u>3</u> levels

at each level 27 quantities to evaluate

(each one involves 2 additions / 2 multiplications)

$3 \times 27 = 27 \log_3 27 \rightarrow N \log_e N$

Worksheet 2:

3.) $\Psi_1^1 = A \quad \Psi_2^1 = A \quad \Psi_3^1 = C \quad \Psi_4^1 = 0$

$$\Psi_1^2 = \Psi_2^2 = \Psi_2^1 + \frac{\Delta t K}{\Delta x^2}\left[\Psi_3^1 - \Psi_2^1\right]$$

$$= A + \frac{\Delta t K}{\Delta x^2}\left[C - A\right]$$

$$\Psi_3^1 = C + \frac{\Delta t K}{\Delta x^2}\left[A - 2C\right]$$

Worksheet 3:

$$\Psi_j^n = A_n e^{ikj}$$

$$A_{n+1} \cancel{e^{ikj}} = A_n \cancel{e^{ikj}} + \frac{\kappa \Delta t}{2\Delta x^2} A_{n+1} [2\cos k - 2]$$
$$+ \frac{\kappa \Delta t}{2\Delta x^2} A_n [2\cos k - 2]$$

$$\boxed{A_{n+1} = \frac{1 + \frac{\kappa \Delta t}{\Delta x^2}(\cos k - 1)}{1 - \frac{\kappa \Delta t}{\Delta x^2}(\cos k - 1)} A_n}$$

unconditionally stable since ~~at~~

$$\frac{1 + \frac{\kappa \Delta t}{\Delta x^2}(\cos k - 1)}{1 - \frac{\kappa \Delta t}{\Delta x^2}(\cos k - 1)} \leq 1$$

Worksheet 4: