MATH 671 Particle Methods in Scientific Computing Winter 2007

hw#3 due: Tuesday, April 17

1. The associated Legendre equation, $\frac{1}{\sin\theta}(\sin\theta\, f_\theta)_\theta + (l(l+1) - \frac{m^2}{\sin^2\theta})f = 0$, arises from separation of variables for the Laplace equation in spherical coordinates. Let f_l^m denote a solution of the equation for given values of l and m. Show that $\langle f_l^m, f_{l'}^m \rangle = 0$ for $l \neq l'$, where the inner product is the same as in problem 2a below. (hint: copy the steps showing that eigenvectors corresponding to distinct eigenvalues of a real symmetric matrix are orthogonal.)

2. Derive the following results. Refer to class notes for the definitions of $M_m^\pm$, q_m.

a) $\langle h_1, M_m^- h_2 \rangle = -\langle M_m^+ h_1, h_2 \rangle$ where $\langle h_1, h_2 \rangle = \int_0^\pi h_1(\theta)\, h_2(\theta)\, \sin\theta\, d\theta$, h_1, h_2 : real-valued

b) $h_1 = M_m^- f_{m+1}$, $h_2 = f_{m+1} \Rightarrow q_m = \pm\sqrt{\lambda - m(m+1)}$

3. a) Show that $\int_0^\pi \sin^{2l+1}\theta d\theta = \frac{2^{2l+1}(l!)^2}{(2l+1)!}$. This verifies the formula stated in class, $\Theta_{ll}(\theta) = \sqrt{\frac{(2l+1)!}{2^{2l+1}(l!)^2}} \sin^l\theta$.

b) Write out the spherical harmonics $Y_l^m(\theta, \phi)$ explicitly for $l = 3, m = 0, 1, 2, 3$. Start with $\Theta_{33}(\theta)$ and use the recurrence relation for $\Theta_{l,m-1}(\theta)$ in terms of $\Theta_{l,m}(\theta)$.

c) Find the Legendre polynomial $P_3(u)$ two ways: (i) recurrence relation, starting with $P_0(u) = 1, P_1(u) = u$, (ii) multipole expression, $P_l(u) = \frac{(-1)^l}{l!} r^{l+1} \frac{\partial^l}{\partial z^l}(\frac{1}{r})$.

d) Plot the Legendre polynomials $P_l(\mu)$ on the interval $-1 \leq \mu \leq 1$ for $l = 0, 1, 2, 3, 10$. (hint: you don't need to express $P_{10}(\mu)$ explicitly in order to plot the graph)

4. Find the potential function $\Phi(x)$ due to the given charge distribution $\rho(x)$. Express Φ in both Cartesian coordinates and spherical coordinates.

a) $\rho(x) = \delta(x)$: monopole   b) $\rho(x) = \delta_z(x)$: dipole   c) $\rho(x) = \delta_{zz}(x)$: quadrupole

5. Verify the following formulas which were stated in class in connection with the associated Legendre functions.

a) $\partial_z\left(\frac{x+iy}{r}\right) = \partial_+\left(\frac{z}{r}\right)$ b) $\rho_{m+1} = \frac{1}{r}\rho_m'$, $\rho_0 = \frac{1}{r} \Rightarrow \rho_m = \left(-\frac{1}{2}\right)^m \frac{(2m)!}{m!} \frac{1}{r^{2m+1}}$

6*. Repeat the electrostatic potential calculation from hw#2, problem 5 using the Barnes-Hut treecode with $\theta = 0.25, 0.5, 0.75$. Present a table showing the relative error in the potential. Plot the cpu time and the error vs. N in log-log scales for direct summation and the treecode. Also plot the results in a "phase plane", i.e. for each computation, plot a symbol for which the x-coordinate is the error and the y-coordinate is the cpu time. In developing your code, it is suggested that you first get it working in one space dimension, i.e. assume the particles are located on the x-axis, and then extend the code to three dimensions.

7. Derive the following recurrence relation for the associated Legendre functions.

$$P_n^{m+2}(u) + 2(m+1)\frac{u}{\sqrt{1-u^2}}P_n^{m+1}(u) - (n-m)(n+m+1)P_n^m(u) = 0$$

8. Recall the approximate delta-function used in Ewald summation, $f(x) = \frac{\alpha^3}{\pi^{3/2}} e^{-\alpha^2|x|^2}$. Show that $\int_{\mathbf{R}^3} f(x)\, dx = 1$.

9. Show that $\int_0^\infty \text{erfc}(s) s ds = \frac{1}{4}$. This result was used in the derivation of Ewald summation.

10*. Consider a cluster of N charged particles contained in cube centered at the origin with side L. Assume that the particles have the same charge $q_i = 1$ and that the positions x_i are randomly distributed. Write a code to compute the particle-cluster interaction potential between the given cluster and a particle located at the point $x = (2, 0, 0)$ on the x-axis. Write three versions of the code: (a) direct particle-particle summation, (b) pth order approximation using spherical coordinates, (c) pth order approximation using Cartesian coordinates. The goal of the exercise is to compare the accuracy and efficiency of the two approximate methods. In the case of spherical coordinates, you may use either the standard definition of the spherical harmonics or the Greengard-Rokhlin convention. Consider two cases, $L = 1$ and $L = 2$. For the order of approximation take $p = 2, 4, 6, 8, 10, 12$. Plot the cpu time and the error vs. N in log-log scales for direct summation and the two approximate methods. Also plot the results in a "phase plane", i.e. for each computation, plot a symbol for which the x-coordinate is the error and the y-coordinate is the cpu time. Discuss the results.