NUEN 625 Computational Project

Due Thursday, April 28, 2016

1. Build a computer code to solve the 1-D spherical-geometry S_n equations:

$$\frac{\mu_m}{r^2}\frac{\partial r^2 \psi_m}{\partial r} + \frac{1}{r}\frac{[(\alpha_{m+1/2}\psi_{m+1/2} - \alpha_{m-1/2}\psi_{m-1/2}]}{w_m} + \sigma_t \psi_m =$$

$$\sum_{k=0}^{K} \frac{2k+1}{2}(\sigma_k \phi_k + q_k) P_k(\mu_m)\,, \tag{1}$$

where $r \in [0, r_b]$ with boundary conditions to be defined later, $\{\mu_m, w_m\}_{m=1}^{N}$ denotes a standard S_n quadrature set, σ_ℓ denotes the ℓ'th Legendre cross section coefficient, ϕ_ℓ denotes the ℓ'th Legendre angular flux moment:

$$\phi_\ell = \sum_{k=1}^{N} \psi_k \, P_\ell(\mu_k) \, w_k\,, \tag{2}$$

and q_ℓ denotes the ℓ'th Legendre moment of the inhomogeneous source. It can be convenient to include the starting direction in the cosine array and give it the index $m = 0$. In what follows we assume this convention. Thus, $\mu_0 = -1$. The basic procedure for solving these equations via source iteration is given in the notes. You will have an option for DSA.

2. Generate a uniform mesh.

3. Assume constant cross sections, and a distributed source that is constant within each cell but can vary between cells.

4. Use Gauss quadrature with weights that sum to two. Given such weight normalization, we define a new angular unit. The new unit is a "biradian", and there are 2π steradians per biradian, so

$$\frac{1}{2\pi}\int_{4\pi} d\Omega = 1\ biradian\,.$$

Thus if the angular flux has units of b^{-1}, the scalar flux is given by

$$\phi = \frac{1}{2\pi}\int_{4\pi} \psi\, d\Omega = \int_{-1}^{+1} \psi\, d\mu\,.$$

which obviously corresponds to weights that sum to two.

5. To obtain the scattering source at the starting direction, use the standard polynomial expression:

$$(\mathbf{S}\psi)(\mu_0) = \sum_{k=0}^{K} \frac{2k+1}{2}\sigma_k\phi_k P_k(\mu_0)\,.$$

6. Use a FEM spatial discretization based upon a linear-continuous trial space and a constant weight function in each cell. This approach yields diamond differencing in slabs. Simply use diamond differencing for the starting flux. Your task for the weighted directions will be made far easier if you generate the expressions relating the r-weighted cell average flux and the r^2-weighted cell average flux to the cell edge

fluxes. More specifically, you should generate the γ-coefficients for the r-weighted and r^2-weighted flux averages as follows:

$$\hat{\psi}_i = \gamma_{i,1}\psi_{i+1/2} + (1-\gamma_{i,1})\psi_{i-1/2} = \frac{\int_{r_{i-1/2}}^{r_{i+1/2}} r\tilde{\psi}\, dr}{\int_{r_{i-1/2}}^{r_{i+1/2}} r\, dr}\,,$$

and

$$\psi_i = \gamma_{i,2}\psi_{i+1/2} + (1-\gamma_{i,2})\psi_{i-1/2} = \frac{\int_{r_{i-1/2}}^{r_{i+1/2}} r^2\tilde{\psi}\, dr}{\int_{r_{i-1/2}}^{r_{i+1/2}} r^2\, dr}\,,$$

using the trial space expression for the angular flux:

$$\tilde{\psi} = \psi_{i+1/2}\left(\frac{r - r_{i-1/2}}{h_i}\right) + \psi_{i-1/2}\left(\frac{r_{i+1/2-r}}{h_i}\right)\,.$$

remember that the r-weighted angular fluxes must be used in the angular derivative term. This is so for the starting direction flux even though diamond-difference in space is assumed to solve for the starting direction fluxes themselves. It is also true that the diamond-difference source must be used in the starting direction equation even though r^2-weighting was assumed to solve Eq. (1).

7. Input should include:

   (a) The outer radius of the sphere, r_b.

   (b) Number of directions (even only).

   (c) Number of cells.

(d) Source type (constant isotropic distributed source / right isotropic boundary flux / right anisotropic boundary flux/ both 1 and 2/both 1 and 3). An anisotropic flux is defined to be non-zero at μ_1 (the direction closest to $\mu = -1$) and zero at all the other incident directions. Set the starting flux via constant interpolation for the S_2 case:

$$\psi_0 = \psi_1 \,,$$

and via linear interpolation for all other S_n orders:

$$\psi_0 = \psi_1 \frac{\mu_0 - \mu_2}{\mu_1 - \mu_2} + \psi_2 \frac{\mu_0 - \mu_1}{\mu_2 - \mu_1} \,,$$

Set the starting flux to zero if the interpolation yields a negative value.

(e) Source normalization method (point value / integrated source value).

(f) Source normalization values. For point normalization, define the zeroth Legendre moment of the source, q_0 $(p/cm^3 - s)$, and/or the zeroth Legendre moment of the incident angular flux, ϕ_0 $(p/cm^2 - s)$. Thus, $q_m = q_0/2$, all μ_m; and $\psi_m = \phi_0/2$, $\mu_m < 0$. For integral normalization, define the total source (p/s) and/or half-range current $(p/cm^2 - s)$.

(g) σ_a (cm^{-1}) and σ_t (cm^{-1}).

(h) P_n scattering order, K.

(i) If $K > 0$, anisotropic cross section coefficients.

(j) Acceleration (none/DSA).

(k) Convergence tolerance. Terminate iterations when the maximum pointwise relative error in the cell-centered scalar flux is less than the tolerance, τ. The relative change in the cell-centered scalar flux in cell i is given by

$$\delta\phi_{i,r}^{\ell+1} = \left| \frac{\phi_i^{\ell+1} - \phi_i^{\ell}}{\phi_i^{\ell+1}} \right| ,$$

where ℓ is the iteration index. The relative error in the cell-average scalar flux in cell i is approximately given by

$$\epsilon_{i,r}^{\ell+1} = \frac{\delta\phi_{i,r}^{\ell+1}}{1 - \tilde{\rho}^{\ell+1}} ,$$

where $\tilde{\rho}$ is a computational estimate of the iterative spectral radius:

$$\tilde{\rho}^{\ell+1} = \frac{\sum_{i=1}^{N_c} |\phi_i^{\ell+1} - \phi_i^{\ell}|}{\sum_{i=1}^{N_c} |\phi_i^{\ell} - \phi_i^{\ell-1}|} .$$

So the iterations should be terminated when

$$\max_i \left| \delta\phi_{i,r}^{\ell+1} \right| < \tau \, (1 - \tilde{\rho}^{\ell+1}) .$$

You should also define a maximum number of iterations that can be performed to prevent the code from running indefinitely.

8. The spatial cell-edge values of the Legendre flux moments should be saved rather than the volume-averaged moments because of the need to construct the diamond-difference source for the starting direction. Similarly, all of the spatial cell-edge starting-direction fluxes should be saved because of the need to construct the r-weighted average flux in the angular derivative term. The angular fluxes can be discarded after their contributions to the Legendre moments have been made. The full angular flux should be saved at the right boundary.

9. Derive a nearly-consistent diffusion equation for use in DSA as follows:

   - Take the zeroth and first moments of the spatially-analytic S_n equations to confirm that one obtains the standard P_1 equations.
   - Apply the linear-continuous FEM method to these equations remembering that r^2 weighting must be applied to both equations for consistency with the S_n discretization.
   - Add the balance equations for cells i and $i+1$, and make the following approximation:

     $$A_{i+3/2}J_{i+3/2} - A_{i-1/2}J_{i-1/2} \approx 2(A_{i+1}J_{i+1} - A_iJ_i)\,,$$

     where J_i is the volume-averaged current for cell i and A_i is the arithmetic average of $A_{i+1/2}$ and $A_{i-1/2}$.

- With this approximation, you will be able to eliminate the currents from the balance equation and obtain a diffusion equation.

10. Describe the DSA algorithm for the analytic transport equation in spherical geometry and show that it results in a conservative accelerated iterate after each iteration if both the scalar flux and the currents are updated with the DSA error estimates. Consider both vacuum and source conditions at the right boundary. As part of the DSA algorithm in your code, update the outgoing angular fluxes at the right boundary in addition to the cell-edge scalar fluxes to ensure *global* conservation after *each* iteration. This is achieved by using a Marshak condition for the diffusion equation consistent with the quadrature formula. For instance at the right boundary:

$$\frac{\delta\phi\langle u\rangle - \delta J}{2} = 0\,,$$

where

$$\langle\mu\rangle = \sum_{\mu_m>0} \mu_m w_m\,.$$

11. Output should include:

    (a) Volume-weighted scalar fluxes, and a balance table including total inhomogeneous source rate, total right inflow rate, total right outflow rate, total absorp-

tion rate, and a balance measure:

$$bal = \left| \frac{total\ source\ rate - total\ sink\ rate}{total\ source\ rate} \right|,$$

where all rates have units of p/s.

12. Your balance table should show round-off conservation after each iteration if you use DSA. This is a very important property for code verification. To ensure that this happens it is easiest to update the outgoing angular fluxes at the right boundary, which will effectively update the outgoing half-range flux:

$$\psi_m^{\ell+1} = \psi_m^{\ell+1/2} + \frac{\delta\phi^{\ell+1/2} + 3\,\delta J^{\ell+1/2}\mu_m}{2}, \quad \text{for } \mu_m > 0.$$

13. Remember to set only the incoming quadrature fluxes and the starting flux on the outer boundary. All remaining angular cell-edge fluxes exist only as r-weighted spatial averages within each cell and do not exist at the spatial cell edges.

14. All fluxes at the origin should be set equal to the starting direction flux. This makes the FEM method for the incoming quadrature directions in the first cell invalid because for these directions, one knows both spatial inflow and outflow fluxes, $\psi_{1/2,m}$ and $\psi_{3/2,m}$, $\mu_m < 0$. One wants to solve the balance equation for $\hat{\psi}_{1,m}$ and $\psi_{1,m}$ to maintain conservation, but a relationship between the two is needed to close the system. Since both the inflow and outflow are known, one can use the spatial-weighted

diamond expressions to compute the ratio of $\hat{\psi}_i$ to ψ_i, i.e., compute a coefficient, $\tilde{\gamma}_{i,m}$, such that $\hat{\psi}_{1,m} = \tilde{\gamma}_{i,m}\psi_{i,m}$, and use this ratio to close the system.

15. Thus, for all but the starting flux and the incoming directions in the first cell, you should:

    (a) Use the angular weighted-diamond relationship to eliminate $\hat{\psi}_{i,m+1/2}$ from the balance equation.

    (b) Use the spatial weighted-diamond schemes to eliminate $\hat{\psi}_{i,m}$ and $\psi_{i,m}$ from the balance equation.

    (c) Solve the balance equation for the spatial outflow: $\psi_{i-1/2,m}$ if $\mu < 0$ and $\psi_{i+1/2,m}$ if $\mu > 0$.

    (d) Use the spatial and angular weighted-diamond relationships to solve for the cell averages, $\hat{\psi}_{i,m}$ and $\psi_{i,m}$, and the angular outflow $\hat{\psi}_{i,m+1/2}$, respectively.

16. For the incoming directions in the first cell, you should

    (a) Set $\psi_{1/2,m} = \psi_{1/2,1/2}$, for all μ_m.

    (b) Use the angular weighted-diamond relationship to eliminate $\hat{\psi}_{i,m+1/2}$ from the balance equation.

    (c) Compute $\tilde{\gamma}_{i,m}$ and use it to eliminate $\hat{\psi}_{1,m}$ from the balance equation.

(d) Solve the balance equation for $\psi_{i,m}$.

(e) Use the ratio to solve for $\hat{\psi}_{1,m}$.

(f) Use the angular weighted-diamond relationship to solve for $\tilde{\psi}_{1,m+1/2}$.

17. The following problems should be performed to help verify your code.

(a) $r_b = 1\ cm$, $\sigma_t = 1\ cm^{-1}$, $\sigma_a = 1\ cm^{-1}$, incident isotropic right boundary flux with an incoming partial current of 1 $(p/cm^2 - s)$, S_4 quadrature. Plot the scalar flux solutions using 50, 100, and 200 cells, and tabulate the balance parameters. Compute the order of spatial convergence as follows:

$$\xi = \frac{|L_{50} - L_{100}|}{|L_{100} - L_{200}|},$$

where L_k denotes the outflow rate (p/s) for the calculation with k cells, and ξ approximates the factor by which the error is reduced when the cell width is reduced by a factor of two. Since the spatial discretization scheme is second order, ξ should be equal to four.

(b) $r_b = 1\ cm$, $\sigma_t = 3\ cm^{-1}$, $\sigma_a = 1\ cm^{-1}$, isotropic scattering, incident right boundary flux $\phi_0 = q_0/\sigma_a$ $(p/cm^2 - s)$, a unit distributed source $q_0 = 1$ $(p/cm^3 - s)$, S_8 quadrature, 100 cells, and a convergence tolerance of 10^{-4}. The scalar flux solution to this problem is analytic: $\phi = q/\sigma_a$ $(p/cm^2 - s)$. Plot the numerical

and analytic scalar flux solutions as a function of position. Tabulate the balance parameters.

(c) Repeat Problem 1 with $\sigma_t = 2\ cm^{-1}$, P_3 anisotropic scattering with all Legendre cross-section coefficients equal to $\sigma_s = 1\ cm^{-1}$. Use a convergence tolerance of 10^{-4}. The solution should be very nearly equal to that of Problem 1 because the cross section expansion coefficients correspond to a differential scattering cross section given by $\delta(\mu_s - 1)$, which is analytically equivalent to no scattering at all. In slab geometry with Gauss quadrature, the treatment of such scattering is exact, but this is not the case in spherical geometry because of the starting direction. Compare the two scalar flux solutions in a plot, and compare the balance parameters in a table.

(d) $r_b = 1\ cm$, $\sigma_t = 30\ cm^{-1}$, $\sigma_a = 0\ cm^{-1}$, isotropic scattering, vacuum right boundary condition, a unit distributed source $q_0 = 1\ (p/cm^3 - s)$, S_8 quadrature, 100 cells, and a convergence tolerance of 10^{-4}. The scalar flux solution will essentially be equal to the corresponding analytic diffusion solution with Marshak boundary conditions computed with the S_8 quadrature set. Use DSA. The problem should require about 4-6 iterations. Plot the numerical and diffusion scalar flux solutions as a function of position. Tabulate the balance parameters after each iteration.

18. In summary, your submission should consist of the following:

    (a) Your derivation of the discrete DSA diffusion equation starting from the analytic P_1 equations for $\delta\phi$ and δJ assuming a vacuum boundary condition at the right boundary and a reflective condition at the left boundary. Your final result should consist of a left boundary equation, an interior-mesh equation, and a right boundary equation.

    (b) Your demonstration that the DSA-accelerated transport iterate will be conservative after each iteration.

    (c) The output and plots from each of the four test problems as described earlier.