NE-860: Numerical Transport

Homework 4
Date: 3/15/2017
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1) Starting from the 1-D transport equation with arbitrary anisotropic scattering and an isotropic source, derive the P_3 equations. Additionally, derive the Marshak vacuum conditions for arbitrary left and right boundaries in a slab. Are the consistent with vacuum conditions in P_1 theory?

Solution:

Starting from the mono energetic transport equation in slab geometry with arbitrary angular dependence of scattering and and isotropic source.

$$\mu\frac{\partial\psi}{\partial x} + \Sigma_t(x)\psi(x,\mu) = \int_0^{2\pi} d\phi' \int_{-1}^{1} d\mu' \Sigma_s(x,\mu_0)\psi(x,\mu') + S(x) \tag{1}$$

expand the angular flux

$$\psi(x,\mu) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi}\psi_n(x)P_n(\mu) \tag{2}$$

where

$$\psi_n(x) = 2\pi \int_{-1}^{1} \psi(x,\mu)P_n(\mu)d\mu \tag{3}$$

Before substitution simplify equation 1

$$\int_0^{2\pi} d\phi' \int_{-1}^{1} d\mu' \Sigma_s(x,\mu_0)\psi(x,\mu') = \int_0^{2\pi} d\phi' \int_{-1}^{1} d\mu' \sum_{l=0}^{\infty} \frac{2l+1}{4\pi}\Sigma_{sl}(x)P_l(\mu_0)\psi(x,\mu') \tag{4}$$

Make use of the Legendre addition theorem

$$P_l(\mu_0) = P_l(\mu)P_l(\mu') + 2\sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P_l^m(\mu)P_l^m(\mu')\cos(m(\phi-\phi')) \tag{5}$$

where $P_l^m(\mu)$ are the associated Legendre polynomials defined as

$$P_l^m(\mu) = \sqrt[2]{(1-\mu^2)^m}\frac{d^m P_l}{d\mu^m} \tag{6}$$

substitute this in to get

$$\int_0^{2\pi} d\phi' \int_{-1}^{1} d\mu' \sum_{l=0}^{\infty} \frac{2l+1}{4\pi}\Sigma_{sl}(x)P_l(\mu_0)\psi(x,\mu') = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi}\Sigma_{sl}(x) + \int_{-1}^{1} d\mu'\psi(x,\mu') \int_0^{2\pi} d\phi' \Bigg(P_l(\mu)P_l(\mu') + 2\sum_{m=1}^{l} \frac{(l-m)!}{(l+m)!} P_l^m(\mu)P_l^m(\mu')\cos(m(\phi-\phi'))\Bigg)$$

Since $\cos(m(\phi - \phi')) = 0$ We get the equation

$$\begin{aligned}
&\int_0^{2\pi} d\phi' \int_{-1}^{1} d\mu' \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl}(x) P_l(\mu_0) \psi(x, \mu') \\
&= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl}(x) + \int_{-1}^{1} d\mu' \psi(x, \mu') \int_0^{2\pi} d\phi' \Big(P_l(\mu) P_l(\mu') \Big) \\
&= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl}(x) P_l(\mu) \Big(2\pi \int_{-1}^{1} d\mu' \psi(x, \mu') P_l(\mu') \Big) \\
&= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl}(x) P_l(\mu) \psi_l(x)
\end{aligned}$$

Substitute the above as the scattering term in equation 1.

$$\sum_{n=0}^{\infty} \frac{2n+1}{4\pi} P_n(\mu) \Big(\mu \frac{\partial \psi_n(x)}{\partial x} + \Sigma_t(x) \psi_n(x) \Big) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \Sigma_{sn}(x) P_n(\mu) \psi_n(x) + S_n(x) \tag{7}$$

Using the Legendre recurrence relation we can express $\mu P_n(\mu)$ as

$$\mu P_n(\mu) = \frac{1}{2n+1} \Big((n+1) P_{n+1}(\mu) + n P_{n-1}(\mu) \Big) \tag{8}$$

Substitute equation 8 into equation 7 to get

$$\begin{aligned}
\sum_{n=0}^{\infty} \Bigg(\Big((n+1) P_{n+1}(\mu) + n P_{n-1}(\mu) \Big) \frac{\partial \psi_n(x)}{\partial x} + (2n+1) P_n(\mu) \Sigma_t(x) \psi_n(x) \Bigg) \\
= \sum_{n=0}^{\infty} (2n+1) \Sigma_{sn}(x) P_n(\mu) \psi_n(x) + \sum_{n=0}^{\infty} 4\pi S_n(x)
\end{aligned}$$

To obtain orthogonality we multiply the above equation by $\frac{2m+1}{2} P_m$ and integrate over $-1 \leq \mu \leq 1$

$$\int_{-1}^{1} d\mu \Bigg(\sum_{n=0}^{\infty} \frac{2m+1}{2} P_m(\mu) \Big((n+1) P_{n+1}(\mu) \frac{\partial \psi_n}{\partial x} + n P_{n-1}(\mu) \frac{\partial \psi_n}{\partial x} \Big) \Bigg) = m \frac{\partial \psi_{m-1}}{\partial x} + (m+1) \frac{\partial \psi_{m+1}}{\partial x} \tag{9}$$

and

$$\int_{-1}^{1} d\mu \frac{2m+1}{2} P_m(\mu) (2m+1) P_n(\mu) \Sigma_t(x) \psi_n(x) = (2m+1) \Sigma_t(x) \psi_m(x) \tag{10}$$

Combining the scattering and source terms together

$$\begin{aligned}
\frac{m+1}{2m+1} \frac{\partial \psi_{m+1}}{\partial x} + \frac{m}{2m+1} \frac{\partial \psi_{m-1}}{\partial x} + \Sigma_t(x) \psi_m(x) \\
= \Sigma_{sm}(x) \psi_m(x) + S_m(x), m = 0.....\infty
\end{aligned}$$

From this equation now we may define the P_N equations up to $N = 3$

$$\boxed{N = 0 \qquad \frac{d\phi_1}{dx} + \Sigma_t(x)\phi_0(x) = \Sigma_{s0}\phi_0 + S_0}$$

$$\boxed{N = 1 \qquad \frac{2}{3}\frac{d\phi_2}{dx} + \frac{1}{3}\frac{d\phi_0}{dx} + \Sigma_t(x)\phi_1(x) = \Sigma_{s1}\phi_1 + S_1}$$

$$\boxed{N = 2 \qquad \frac{3}{5}\frac{d\phi_3}{dx} + \frac{2}{5}\frac{d\phi_1}{dx} + \Sigma_t(x)\phi_2(x) = \Sigma_{s2}\phi_2 + S_2}$$

$$\boxed{N = 3 \qquad \frac{3}{7}\frac{d\phi_2}{dx} + \Sigma_t(x)\phi_3(x) = \Sigma_{s3}\phi_3 + S_3}$$

Marshak Conditions: The Marshak condition places a linit on the odd moements of the P_n expansion, as the odd moments drive net flow in angular space. For a boundary condition, we may write

$$\psi(x_l), \mu) = B_L(\mu), \qquad \mu > 0 \tag{11}$$

The Marshak condition may then be written as

$$\int_0^1 \psi(x_L, \mu) P_l(\mu) d\mu \tag{12}$$

For the P_3 boundary conditions on the left boundary equation 12 becomes

$$\boxed{\int_0^1 \frac{1}{2}(5\mu^3 - 3\mu)\psi(x_L, \mu)d\mu}$$

and for the right hand side

$$\boxed{\int_- 1^0 \frac{1}{2}(5\mu^3 - 3\mu)\psi(x_L, \mu)d\mu}$$

2) For this problem, consider a homogeneous slab with cross sections defined in the table:

Σ_T	$1.0\ cm^{-1}$
Σ_{S0}	$0.5\ cm^{-1}$
Σ_{S1}	??? cm^{-1}
Σ_A	$0.5\ cm^{-1}$

The slab is 10cm in width. At the left boundary is a unit incident particle current. Use a mesh-centered diffusion approximation to solve this problem for the cases $\Sigma_{s1} = 0, 0.1$, and $-0.1cm^{-1}$. Plot the resulting fluxes together, and list the outgoing partial current from the right boundary for each. Use a constant Δx in your discretization that is sufficiently small to capture the outgoing convergence to wihin 0.1% of the reference value of the isotropic scattering case (which, ofcourse, you can determine analytically).

Solution:

In this problem we used the Mesh-Centered Diffusion Approximation to determine the flux going through a 10cm slab for different values of SigmaS1. To do this we defined a multiplication matrix L and a solution matrix S by expanding the diffusion equation. The Matrix for L is a tridiagonal matrix. For everywhere except the boundary the diagonals are defined by

$$L[i,j] = 2(\frac{D}{\Delta_x}) + \Sigma_a$$

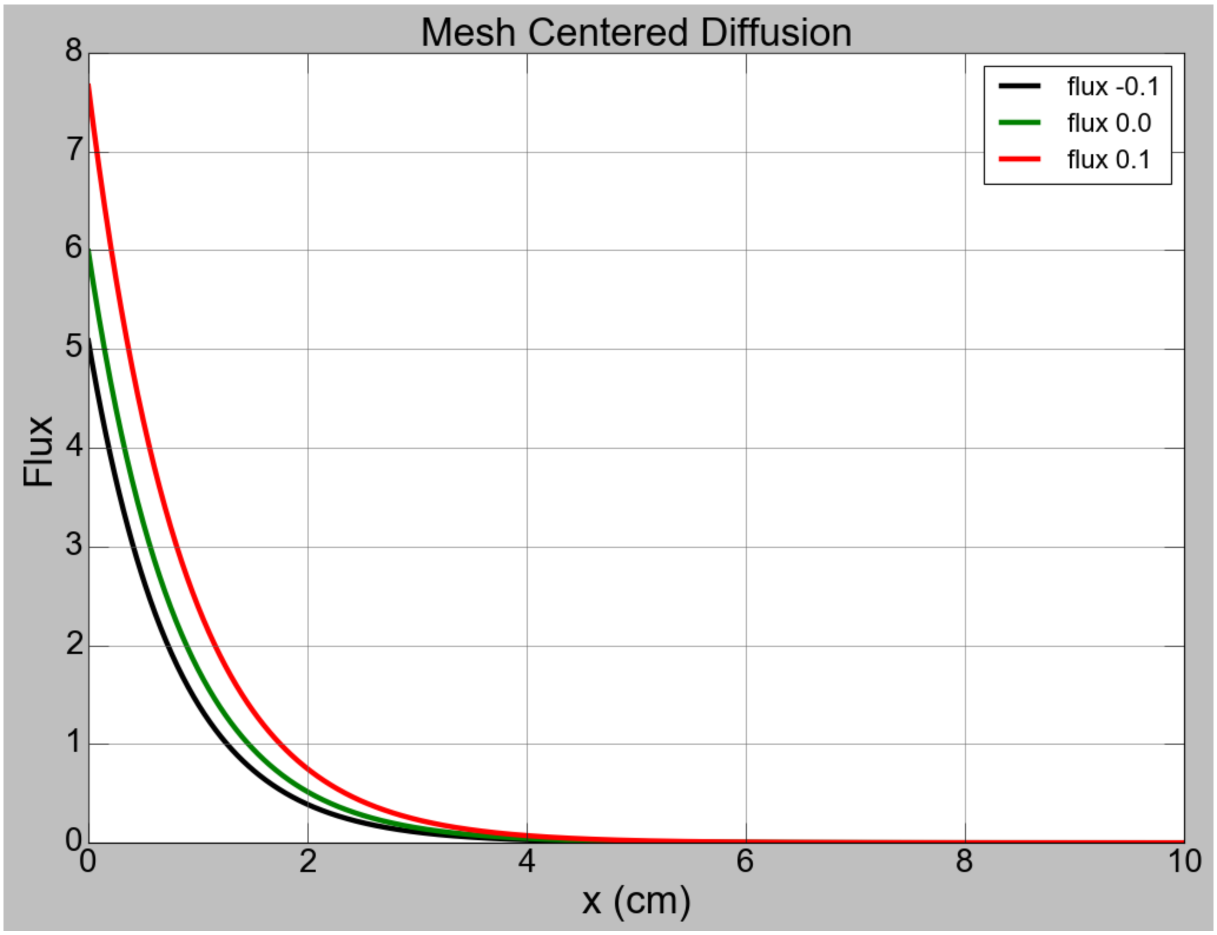
The adjacent components to the left and right of the diagonal are defined by

$$\frac{-D}{\Delta_x}$$

At the boundaries, we assumed a vacuum condition, i.e. $J_i n = 0$ This is defined as equation 10.23 in the text as

$$\phi_x(x_{i\pm 1/2}, y_j, z_k) = \frac{2D_{1jk}\phi_{1,j,k}}{(4D + \Delta_x)\Delta_x}$$

The source term only contributes at the left boundary, therefore we make a source vector with the first component (the left) being S/Δ_x where S was taken to be unity. 1000 points for x were ran and the results were graphed. The graph is shown below. At the right hand boundary, the flux values were tabulated. The flux values for SigmaS1 = -0.1, 0.0, and 0.1 are shown respectively

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[   5.31270050e-07]
[   1.40599933e-06]
[   4.54632061e-06]
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3) You've already become familiar with the Legendre polynomials, and from class, you've learned that the zeros of $P_{N+1}(\mu)$ are the quadrature points for an N-point Gauss-Legendre quadrature. Take the following as true :

- $(l+1)P_{l+1}(x) - (2l+1)xP_l(x) + lP_{l-1}(x) = 0$

- $(l+1)P_{l+1}(x) - (2l+1)xP_l(x) + lP_{l-1}(x) = 0$

- The ith point for an N-point quadrature is approximated by

$x_i \approx \cos\left(\frac{\pi(i-0.25)}{N+0.5}\right)\left(1 - \frac{1}{8}(N^{-2} - N^{-3})\right)$

Now, do the following:

1: Verify that these expressions are correct by direct comparison to known polynomials, their derivatives, and their zeros.
2: Write a function that evaluates $P_l(x)$ for any value of $l \geq 0$ and $x \in [-1, 1]$.
3: Write a function that evalueates the derivative $P_l'(x)$ for any values of $l \geq 0$ and $x \in [-1, 1]$.
4: Using the approximate x_i, write a function that applies Newton's method to find the zeros of $P_l(x)$. Compute these for $l = 3, lo = 11$, and $l = 24$.

Solution:

For this problem, I will address the problems in order as given in the problem statement. To verify the functions given I used the Legendre polynomials and their derivatives, which I got from the further problems to check that the end result equals zero. I made a loop that will round to 10 decimal places to remove any floating point errors and checked 1000 cases of x to prove that the equations hold true. To find the Legendre polynomials and their value in the domain -1 to 1. I used a special scipy function within a definition that calculates and solves these polynomials. To find the derivative of the polynomials I used a numpy function polyder that when given the Legendre equations will automatically find the derivatives. For the zeros I made a definition that uses a special built in newtons method function that will find the roots of the equations given to it. This code may be seen in my github account. The zeros of the values for l=3,11,and 24 can be seen in the figure below.

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Here are the Zeros for N=3
[0.77459666924099291, -2.2587516133581508e-28, -0.7745966692409928]

Here are the Zeros for N=11
[0.97822865814605964, 0.8870625997620144, 0.73015200557388005, 0.51909612920681014,
0.26954315595234524, 0.0, -0.26954315595234524, -0.51909612920681014, -0.73015200557388005,
-0.88706259976201429, -0.97822865814605964]

Here are the Zeros for N=24
[0.99518721999718118, 0.97472855592422281, 0.93827455199987542, 0.88641552700404824,
0.82000198597384277, 0.7401241915785427, 0.64809365193697333, 0.54542147138883923,
0.43379350762604518, 0.31504267969616329, 0.19111886747361634, 0.064056892862605672,
-0.064056892862605727, -0.19111886747361626, -0.31504267969616334, -0.43379350762604513,
-0.54542147138883923, -0.64809365193697333, -0.7401241915785427, -0.82000198597384266,
 -0.88641552700404835, -0.93827455199987542, -0.97472855592422292, -0.99518721999718118
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4) Use the discrete-ordinates method to solve Problem3. Use the same spatial discretization. Use Gauss-Legendre quadrature of 16 angles per half space (often called a S_{32} approximation). For the case of isotropic scattering, what's the analytic expression for the outgoing current?

Solution:

For problem 4 the Discrete Ordinates Method was used with 16 angles per half space to achieve the same answer as in problem 2. This was an iterative process that converged on a solution for the flux values in each cell by performing sweeps. To avoid getting negative flux values, the Step Difference method was used. The code for this method may be seen in my github repository. The graph from this code for SigmaS1=0 is shown below