NE 255: Numerical Simulation in Radiation Transport
Homework #5

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1. The operator form of the Transport Equation is given in Eq. (1).

$$\boldsymbol{L}\psi = \boldsymbol{M}\boldsymbol{S}\phi + \boldsymbol{M}q_e \tag{1}$$

$$\phi = \boldsymbol{D}\psi \tag{2}$$

where $\boldsymbol{L} = \hat{\boldsymbol{\Omega}}\cdot\nabla + \Sigma_t$ is the transport operator, the moment-to-discrete operator $\boldsymbol{M}$ converts harmonic moments into discrete angles, and $\boldsymbol{S}$ is the scattering matrix. Eq. (2) can be used to find the flux moment ϕ given angular flux ψ, where the discrete-to-moment operator $\boldsymbol{D} = \boldsymbol{M}^T\boldsymbol{W} = \sum_{a=1}^{n} Y_{\ell m}^{e/o} w_a$ converts discrete angles into harmonic moments.

Considering the following discretizations ...

- 3 groups ($G = 3$)
- P_2 – number of moments, $N = (N'+1)^2 = 9$, defining N' as being from $P_{N'}$
- S_2 – number of angles, $n = N'(N'+2) = 8$, defining N' as being from $S_{N'}$
- $4 \times 4 \times 4$ mesh ($c = 64$)
- Diamond Difference

(a) The matrix and vector dimensions in the transport equation are given by α and β, defined as:

$$\begin{aligned}\alpha &= G \times n \times c \times u \\ &= (\#\text{ of groups})(\#\text{ of angles})(\#\text{ of mesh cells})(\#\text{ of unknowns per cell}) \\ &= 3 \times 8 \times 64 \times 1 = \boxed{1536}\end{aligned}$$

$$\begin{aligned}\beta &= G \times N \times c \times u \\ &= (\#\text{ of groups})(\#\text{ of moments})(\#\text{ of mesh cells})(\#\text{ of unknowns per cell}) \\ &= 3 \times 9 \times 64 \times 1 = \boxed{1728}\end{aligned}$$

The dimensions for each matrix and vector in Eqs. (1) and (2) are given in Table 1.

Table 1: Matrix and vector dimensions

Matrix/vector	General dimensions	Values for this problem
$\boldsymbol{L}$	$\alpha \times \alpha$	1536×1536
$\boldsymbol{M}$	$\alpha \times \beta$	1536×1728
$\boldsymbol{S}$	$\beta \times \beta$	1728×1728
$\boldsymbol{D}$	$\beta \times \alpha$	1728×1536
ψ	$\alpha \times 1$	1536×1
q_e	$\beta \times 1$	1728×1
ϕ	$\beta \times 1$	1728×1

(b) Moment-to-discrete operator $\boldsymbol{M}$

$$\boldsymbol{M} = \begin{bmatrix} \boldsymbol{M}_{11} & 0 & 0 \\ 0 & \boldsymbol{M}_{22} & 0 \\ 0 & 0 & \boldsymbol{M}_{33} \end{bmatrix}$$

$[\boldsymbol{M}]_{gg} =$

$$\begin{bmatrix} Y_{00}^e(\hat{\boldsymbol{\Omega}}_1) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_1) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_1) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_1) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_1) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_1) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_1) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_1) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_1) \\ Y_{00}^e(\hat{\boldsymbol{\Omega}}_2) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_2) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_2) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_2) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_2) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_2) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_2) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_2) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_2) \\ Y_{00}^e(\hat{\boldsymbol{\Omega}}_3) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_3) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_3) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_3) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_3) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_3) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_3) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_3) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_3) \\ Y_{00}^e(\hat{\boldsymbol{\Omega}}_4) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_4) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_4) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_4) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_4) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_4) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_4) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_4) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_4) \\ Y_{00}^e(\hat{\boldsymbol{\Omega}}_5) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_5) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_5) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_5) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_5) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_5) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_5) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_5) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_5) \\ Y_{00}^e(\hat{\boldsymbol{\Omega}}_6) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_6) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_6) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_6) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_6) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_6) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_6) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_6) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_6) \\ Y_{00}^e(\hat{\boldsymbol{\Omega}}_7) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_7) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_7) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_7) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_7) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_7) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_7) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_7) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_7) \\ Y_{00}^e(\hat{\boldsymbol{\Omega}}_8) & Y_{10}^e(\hat{\boldsymbol{\Omega}}_8) & Y_{11}^o(\hat{\boldsymbol{\Omega}}_8) & Y_{11}^e(\hat{\boldsymbol{\Omega}}_8) & Y_{20}^e(\hat{\boldsymbol{\Omega}}_8) & Y_{21}^o(\hat{\boldsymbol{\Omega}}_8) & Y_{21}^e(\hat{\boldsymbol{\Omega}}_8) & Y_{22}^o(\hat{\boldsymbol{\Omega}}_8) & Y_{22}^e(\hat{\boldsymbol{\Omega}}_8) \end{bmatrix}$$

Scattering matrix $\boldsymbol{S}$

$$\boldsymbol{S} = \begin{bmatrix} [\boldsymbol{S}]_{11} & [\boldsymbol{S}]_{12} & [\boldsymbol{S}]_{13} \\ [\boldsymbol{S}]_{21} & [\boldsymbol{S}]_{22} & [\boldsymbol{S}]_{23} \\ [\boldsymbol{S}]_{31} & [\boldsymbol{S}]_{32} & [\boldsymbol{S}]_{33} \end{bmatrix}$$

$$[\boldsymbol{S}]_{21} = \begin{bmatrix} \Sigma_{s0}^{21} & & & & & & & 0 \\ & \Sigma_{s1}^{21} & & & & & & \\ & & \Sigma_{s1}^{21} & & & & & \\ & & & \Sigma_{s1}^{21} & & & & \\ & & & & \Sigma_{s1}^{21} & & & \\ & & & & & \Sigma_{s1}^{21} & & \\ & & & & & & \Sigma_{s1}^{21} & \\ & & & & & & & \Sigma_{s1}^{21} \\ 0 & & & & & & & \end{bmatrix}$$

Angular flux vector ψ

$$\psi = \begin{pmatrix} [\psi]_1 & [\psi]_2 & [\psi]_3 \end{pmatrix}^T$$

$$[\psi]_1 = \begin{pmatrix} \psi_1^1 & \psi_2^1 & \dots & \psi_8^1 \end{pmatrix}^T$$

Flux moment vector ϕ

$$[\phi]_1 = \begin{pmatrix} \phi_{00}^1 & \phi_{10}^1 & \vartheta_{11}^1 & \phi_{11}^1 & \phi_{20}^1 & \vartheta_{21}^1 & \phi_{21}^1 & \vartheta_{22}^1 & \phi_{22}^1 \end{pmatrix}^T$$

(c) The discrete-to-moment operator $\boldsymbol{D} = \boldsymbol{M}^T\boldsymbol{W}$ where $\boldsymbol{W}$ is an $n \times n$ matrix of the weights for the chosen S_N quadrature set.

$$\boldsymbol{D} = \begin{bmatrix} \boldsymbol{D}_{11} & 0 & 0 \\ 0 & \boldsymbol{D}_{22} & 0 \\ 0 & 0 & \boldsymbol{D}_{33} \end{bmatrix} = \begin{bmatrix} \boldsymbol{M}_{11}^T & 0 & 0 \\ 0 & \boldsymbol{M}_{22}^T & 0 \\ 0 & 0 & \boldsymbol{M}_{33}^T \end{bmatrix} \boldsymbol{W}$$

$$\boldsymbol{D}_{gg} = \boldsymbol{M}_{gg}^T = \begin{bmatrix} Y_{00}^e(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{00}^e(\hat{\boldsymbol{\Omega}}_8) \\ Y_{10}^e(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{10}^e(\hat{\boldsymbol{\Omega}}_8) \\ Y_{11}^o(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{11}^o(\hat{\boldsymbol{\Omega}}_8) \\ Y_{11}^e(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{11}^e(\hat{\boldsymbol{\Omega}}_8) \\ Y_{20}^e(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{20}^e(\hat{\boldsymbol{\Omega}}_8) \\ Y_{21}^o(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{21}^o(\hat{\boldsymbol{\Omega}}_8) \\ Y_{21}^e(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{21}^e(\hat{\boldsymbol{\Omega}}_8) \\ Y_{22}^o(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{22}^o(\hat{\boldsymbol{\Omega}}_8) \\ Y_{22}^e(\hat{\boldsymbol{\Omega}}_1) & \dots & Y_{22}^e(\hat{\boldsymbol{\Omega}}_8) \end{bmatrix} \boldsymbol{W}$$

(d) We don't form an $\boldsymbol{L}$ matrix because we don't need to; rather than storing the matrix, we implement the action of applying $\boldsymbol{L}$ through diamond differences.

(e) The operator form of the Transport Equation from Eq. (1) can be rewritten in the form $\boldsymbol{A}x = b$ using Eq. (2).

$$
\begin{aligned}
\boldsymbol{L}\psi &= \boldsymbol{M}\boldsymbol{S}\phi + \boldsymbol{M}q_e \\
\boldsymbol{L}\left(\boldsymbol{D}^{-1}\phi\right) &= \boldsymbol{M}\boldsymbol{S}\phi + \boldsymbol{M}q_e \\
\phi &= \boldsymbol{D}\boldsymbol{L}^{-1}\boldsymbol{M}\boldsymbol{S}\phi + \boldsymbol{D}\boldsymbol{L}^{-1}\boldsymbol{M}q_e \\
\left(\boldsymbol{I} - \boldsymbol{D}\boldsymbol{L}^{-1}\boldsymbol{M}\boldsymbol{S}\right)\phi &= \boldsymbol{D}\boldsymbol{L}^{-1}\boldsymbol{M}q_e \\
\boldsymbol{A}x &= b
\end{aligned}
$$

2.

- $x_0 = 0.0$, $x_1 = 2.0$, $h = 0.1$
- $\alpha = 0.5$
- $\mu_a = \pm[0.2, 0.5, 0.7]$
- $\Sigma_{t1} = 0.5$, $\Sigma_{t2} = 0.8$, $\Sigma_{t3} = 1.0$
- $\Sigma_s^{gg'}$ given in Table 2
- $q_{e1} = 1.5$, $q_{e2} = 0.0$, $q_{e3} = 0.2$
- left boundary condition is 0.5 incoming in group 1, zero otherwise

Table 2: Scattering Cross Section Values

		g'		
		1	2	3
	1	0.1	0.0	0.0
g	2	0.3	0.1	0.1
	3	0.1	0.3	0.3

The discretized Transport Equation for an energy group g is given by Eq. (3):

$$
\frac{\mu_a}{h_i}\left(\psi^g_{a,i+1/2} - \psi^g_{a,i-1/2}\right) + \Sigma^g_{t,i}\psi^g_{a,i} = 2\sum_{a=1}^{N} w_a \sum_{g'=1}^{G} \Sigma^{gg'}_{s,i}(a' \to a)\psi^{g'}_{a',i} + \frac{q_e}{n} \tag{3}
$$

Jacobi iteration is an order independent method that uses values from previous iterations to calculate values for the current iteration.

$$
\boldsymbol{L}\psi^{j+1}_g = [\boldsymbol{M}][\boldsymbol{S}]_{gg}[\phi]^j_g + [\boldsymbol{M}]\left(\sum_{g'=1}^{g-1}[\boldsymbol{S}]_{gg'}[\phi]^j_g + \sum_{g'=g+1}^{G}[\boldsymbol{S}]_{gg'}[\phi]^j_{g'} + [q_e]_g\right) \tag{4}
$$

The rhs of Eq. (3) is the source term for a group g, and can be written more explicitly using Eq. (4):

$$
\begin{aligned}
S^g_i &= \frac{q^g_e}{n} + + \sum_{g'=1}^{G} \Sigma^{gg'}_s \phi^g_i \\
\text{where } \phi^g_i &= 2\sum_{a=1}^{N} w_a \phi^g_{a,i} = \frac{2}{n}\sum_{a=1}^{N} \phi^g_{a,i}
\end{aligned}
$$

This gives a system of three equations, one for each value of g, and therefore three values of angular flux.

It is now possible to find $\psi^g_{a,i}$ for each energy group, applying the same method used in Homework 4. For $\mu > 0$, $\psi_{i-1/2}$ is the incoming flux and $\psi_{i+1/2}$ is the outgoing flux. For $\mu < 0$, $\psi_{i+1/2}$ is the incoming flux and $\psi_{i-1/2}$ is the outgoing flux.

$$\psi^g_{a,i} = \left(\frac{2|\mu|}{h(1 \pm \alpha)}\psi^g_{a,i\mp 1/2} + S^g_i\right) \Bigg/ \left(\frac{2|\mu|}{h(1 \pm \alpha)} + \Sigma^g_t\right)$$
$$\psi^g_{a,i\pm 1/2} = \frac{2}{1 \pm \alpha}\psi^g_{a,i} - \frac{1 \mp \alpha}{1 \pm \alpha}\psi^g_{a,i\mp 1/2}$$

The results are plotted in Fig. 1.

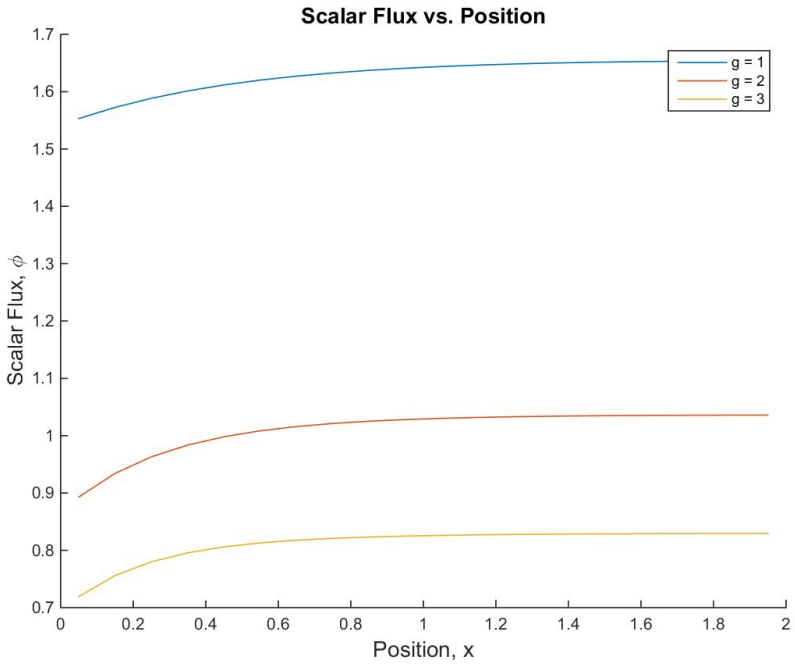

Figure 1: $\phi(x)$ for $g = 1, 2, 3$

Code

```
clear all
close all
clc

% SOURCE CONVERGENCE TOLERANCE
TOL = 1E-4;

% BOUNDARY CONDITIONS
x0 = 0;
x1 = 2;
```

```
psi0 = [0.5, 0.0, 0.0];

% CONSTANTS
sigmaT = [0.5, 0.8, 1.0]';  % total cross section
sigmaS = [...               % scattering cross section
    0.1, 0.0, 0.0;  ...
    0.3, 0.1, 0.1;  ...
    0.1, 0.3, 0.3];
qe = [1.5, 0.0, 0.2];       % external source
G = length(qe);             % # of energy groups

mu = [0.2, -0.2, 0.5, -0.5, 0.7, -0.7]; % angle
n = length(mu);                         %   # of angles

alpha = 0.5;                % alpha

h = 0.1;                    % cell width
N = (x1 - x0) / h;          %   # of cells
x = x0+h/2 : h : x1-h/2;    % mid-cell points
xHalf = x0 : h : x1;        % cell boundary points

qa = qe / n;    % local source
wa = 2 / n;     % weight

% INITIALIZE SOLUTION & CALCULATION VECTORS
psi = zeros(n, N, G);       % angular flux
phi = zeros(1, N, G);       % scalar flux
S = zeros(1, N, G);         % source
Sprev = S;                  % source from previous iteration
dS = S;                     % change in source between iterations

relerr = ones(1:G);     % relative error

%% Until source convergence...
while relerr(1) > TOL && relerr(2) > TOL && relerr(3) > TOL

    %% Iterate over group...
    for g = 1:G

        % Apply boundary condition for first angle
        psiHalf = zeros(1, N+1);    % angular flux @ cell boundaries
        psiHalf(1) = psi0(g);       %   initial condition

        %% Iterate over angle...
        for a = 1:n

            % mu-dependent terms
```

```
            alphaPM = (1 + sign(mu(a)) * alpha);    % plus-minus alpha term
            alphaMP = (1 - sign(mu(a)) * alpha);    % minus-plus alpha term
            C = 2 * abs(mu(a)) / (h * alphaPM);     % constant

            %% Iterate across space...
            for i = 1:N

                % Test for positive or negative angle.
                if mu(a) > 0;   imid = i;       iprev = i;       inext = i+1;
                else            imid = N+1-i;   iprev = N+2-i;   inext = N+1-i;
                end

                % Calculate flux moment.
                phi(1,imid,:) = wa * sum(psi(:,imid,:),1);

                % Source term -- within group
                S(1,imid,g) = qa(g);

                % Source term -- multigroup
                for k = 1:G;
                    S(1,imid,g) = S(1,imid,g) + sigmaS(g,k) * phi(1,imid,k);
                end

                %% ANGULAR FLUX
                psi(a,imid,g) = (C * psiHalf(iprev) + S(imid)) / (C + sigmaT(g));
                psiHalf(inext) = (2 * psi(a,imid,g) - alphaMP * psiHalf(iprev)) /↩
                     alphaPM;

            end
        end

        % SOURCE CONVERGENCE CALCULATIONS
        dS(1,:,g) = abs(S(1,:,g) - Sprev(1,:,g));
        relerr(g) = norm(dS(1,:,g), 'fro') / norm(S(1,:,g), 'fro');
        Sprev(1,:,g) = S(1,:,g);    % make S previous S

    end
end

%% PLOT
f = figure();   % initialize figure

hold on
for g = 1:G
    phi = wa * sum(psi(:,:,g), 1);  % calculate final flux moment
    plot(x, phi);                   % generate plot
end
```

```
hold off

% PLOT SETTINGS
FONTSIZE = 10;
SCALE = 1/0.75;

% LABEL
title('Scalar Flux vs. Position',   'FontSize', FONTSIZE*SCALE);
xlabel('Position, x',               'FontSize', FONTSIZE*SCALE);
ylabel('Scalar Flux, \phi',         'FontSize', FONTSIZE*SCALE);

legend({'g = 1', 'g = 2', 'g = 3'});

% SAVE
saveas(f, 'multigroup', 'jpeg');
```