HW 3 - NE 255 - Lorenzo Vergari

1) **Describe the sweeping process in one dimension (marching through space) along one angle using the diamond difference scheme**

Consider the i-th 1D cell in a 1D grid:

$$x_{i-\frac{1}{2}} \qquad\qquad x_i \qquad\qquad x_{i+\frac{1}{2}}$$

We can integrate the angular flux derivative across the cell as:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial \psi}{\partial x} dx = \psi\left(x_{i+\frac{1}{2}}\right) - \psi\left(x_{i-\frac{1}{2}}\right) \tag{1}$$

Be $\Delta_i = x_{i+1/2} - x_{i-1/2}$ and be $\mu = \cos(\theta)$. In the diamond difference scheme, we have:

$$\psi_i = \frac{1}{2}\left[\psi_{i+\frac{1}{2}} + \psi_{i-\frac{1}{2}}\right] \tag{2}$$

Then, we consider the transport equation for a given angular direction μ:

$$\mu\frac{\partial \psi}{\partial \mathrm{x}} + \Sigma_t\psi = 2\pi\int_0^\infty dE'\int_{-1}^{1} \mathrm{d}\mu'\Sigma_s(\mu', E' \to E, x)\psi + \frac{\chi}{2}\int_0^\infty \nu(\mathrm{E}')\Sigma_f(E', x)\psi dE' + Q \tag{3}$$

Let's integrate the equation across the cell. For the spatial derivative, perform the replacement as for (1) and divide by Δ_i. For the other terms, consider $\int_{x_{i-1/2}}^{x_{i+1/2}} \psi\, dx = \psi_i\Delta_i$.

For simplicity, let's condense the term on the right hand side as S (S_i within the i-th cell)

$$\frac{\mu}{\Delta_i}\left[\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}\right] + \Sigma_{t_i}\psi_i = S_i \tag{4}$$

a.

Be mu>0; we will proceed from left to right in the solution.

Now, suppose to know the flux in the (i-1)- th cell ψ_{i-1}; if we are sweeping in the positive direction, we are interested in computing the angular flux in the cell immediately at the right, i.e. at x_i .

To do so, first we compute the incoming flux at the left shared face $\bar{\psi}_{i-\frac{1}{2}}$, which will be equal in the two cells for continuity, reverting (1) and changing the indices in order to account for the (i-1)th cell:

$$\bar{\psi}_{i-\frac{1}{2}} = 2\psi_{i-1} - \psi_{(i-1)-\frac{1}{2}} \tag{5}$$

Now, we consider the i-th cell and use (1) again to write:

Hence, we perform the replacement in the equation (4) and solve for ψ_i:

$$\psi_i = \frac{S_i + \frac{2\mu}{\Delta_i}\bar{\psi}_{i-\frac{1}{2}}}{\Sigma_{t,i} + \frac{2\mu}{\Delta_i}} \tag{7}$$

In this manner, starting from the boundary condition at the left side of the domain ($x_{\frac{1}{2}}$ for how the indices have been defined here), we manage to sweep across the entire domain one executing the sequence of equations (7) and (6) for i=1,…,N.

b.

If mu<0, let's now proceed from right to left. In this case, our boundary condition will be the $\psi_{N+\frac{1}{2}}$

For a generic i, we can write, with $\bar{\psi}_{i+\frac{1}{2}}$ being the flux incoming in the cell:

$$\psi_{i-\frac{1}{2}} = 2\psi_i - \bar{\psi}_{i+\frac{1}{2}} \tag{8}$$

Next, we consider the integration of the transport equation across the cell:

$$\frac{\mu}{\Delta_i}\left[\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}\right] + \Sigma_{t_i}\psi_i = S_i \tag{9}$$

We replace $\frac{\mu}{\Delta_i}\left[\psi_{i+\frac{1}{2}} - \psi_{i-\frac{1}{2}}\right]$ $with$ $\frac{|\mu|}{\Delta_i}\left[\psi_{i-\frac{1}{2}} - \psi_{i+\frac{1}{2}}\right]$, replace according to (8) and solve for ψ_i:

$$\psi_i = \frac{S_i + \frac{2|\mu|}{\Delta_i}\bar{\psi}_{i+\frac{1}{2}}}{\Sigma_{t,i} + \frac{2|\mu|}{\Delta_i}} \tag{10}$$

And finally we update $\psi_{i-\frac{1}{2}}$ and proceed with the next cell, until the boundary on the right.

c.

At the reflecting boundary on the right side, we take $\mu_2 < 0 \; and \; \mu_1 > 0$:

$$\bar{\psi} \quad (x = x_L, \mu_1) = \psi(x = x_L, \mu_2) \tag{11}$$

Hence, proceeding from left to right, we have:

$$\psi_N(\mu = \mu_1) = \frac{S_N + \frac{2\mu_1}{\Delta_N}\bar{\psi}_{N-\frac{1}{2}}(\mu = \mu_1)}{\Sigma_{t,N} + \frac{2\mu_1}{\Delta_N}} \tag{12}$$

$$\psi_{N+\frac{1}{2}}(\mu = \mu_1) = 2\psi_N(\mu = \mu_1) - \psi_{N-\frac{1}{2}}(\mu = \mu_1) \tag{13}$$

We reflect the angular flux and start to sweep from right to left

$$\psi_{N+\frac{1}{2}}(\mu = \mu_2) = \bar{\psi}_{N+\frac{1}{2}}(\mu = \mu_1) \tag{14}$$

$$\psi_N(\mu = \mu_2) = \frac{S_N + \frac{2|\mu_2|}{\Delta_N}\bar{\psi}_{N+\frac{1}{2}}(\mu = \mu_2)}{\Sigma_{t,N} + \frac{2|\mu_2|}{\Delta_N}} \tag{15}$$

$$\psi_{N-\frac{1}{2}}(\mu = \mu_2) = 2\psi_i(\mu = \mu_2) - \bar{\psi}_{N+\frac{1}{2}}(\mu = \mu_2) \tag{16}$$

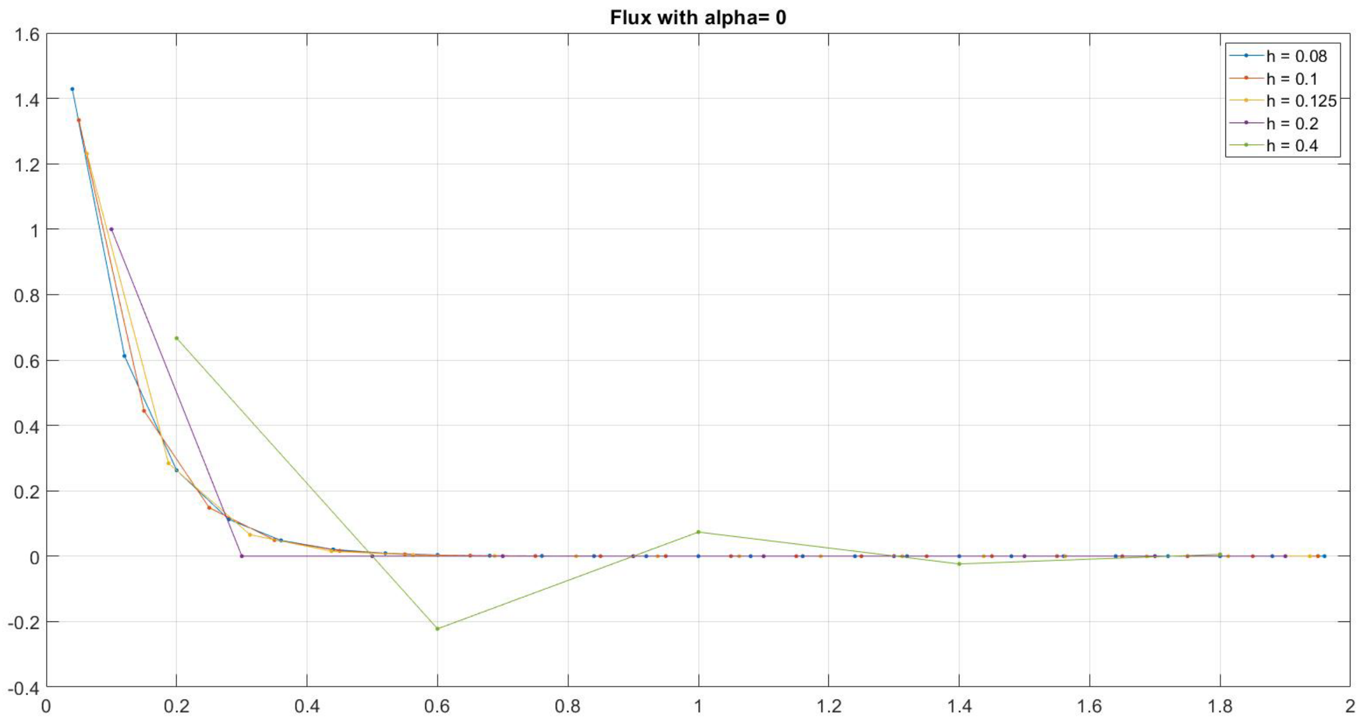
d.

In order to calculate the flux moments, we will need to store the value of the angular flux at the center of the cells (and the location of the cell centers), multiply the angular fluxes by their mu-value, and sum them for each cell. We don't need the value at the interfaces between cells. We need the angular flux boundary condition at the extremes of the mesh, though.

2. **Write some code that implements the 1-D, one-speed, steady state, weighted diamond difference equations; include isotropic scattering and an isotropic external source.**

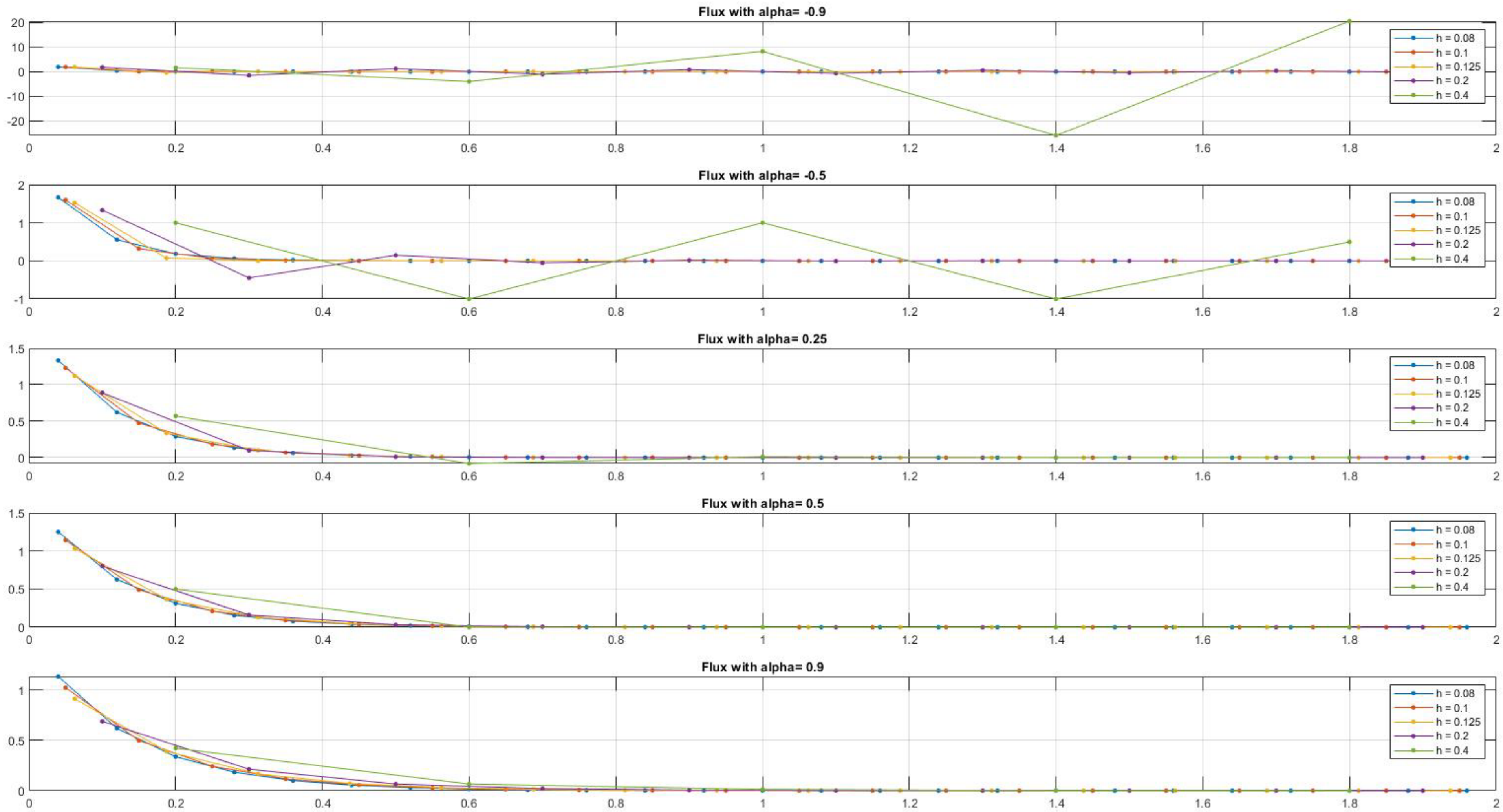
See attached codes.

a)

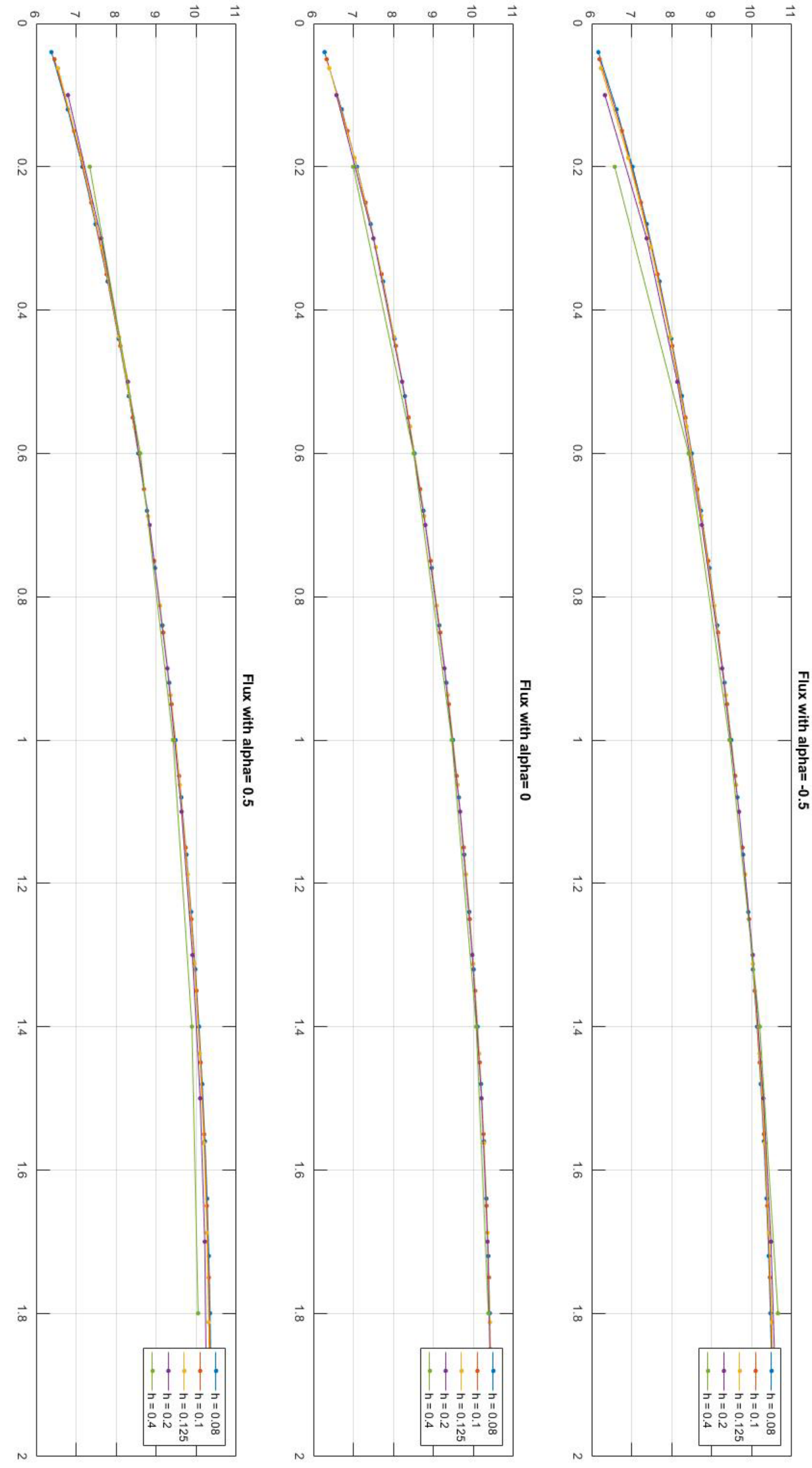


The result is unphysical with the largest mesh spacing, as the scalar flux becomes negative.

b) We see that with negative values of alpha (<0.5), the flux becomes largely negative, and that it is slightly negative for alpha=0.25


Flux with alpha= -0.9
Flux with alpha= -0.5
Flux with alpha= 0.25
Flux with alpha= 0.5
Flux with alpha= 0.9
h = 0.08
h = 0.1
h = 0.125
h = 0.2
h = 0.4

c) We see that now the flux has flipped concavity and it becomes higher when farther away from the boundary



3. **Consider the operator form of the transport equation …**

a) Dimensions of the matrix

Consider the following notation:

- $G = 3$ – number of energy groups
- $n = N(N+2) = \ 8$ – number of discrete angles
- $K = (N+1)^2 = 9$ – number of moments
- $c = 4^3 = 64$ – number of spatial cells
- u =1 - unknowns per cell
- $\alpha = G \times n \times c \times u$ = 1536
- $\beta = G \times K \times c \times u = 1728$

Then, the matrices have the following sizes

$[\mathbf{L}] = (\alpha \times \alpha) = 1536 \times 1536;$

$[\boldsymbol{M}] = (\alpha \times \beta) = 1536 \times 1728;$

$[\boldsymbol{S}] = (\beta \times \beta) = 1728 \times 1728;$

b) Components:

$$[\boldsymbol{M}] = \begin{bmatrix} Y_{00}^e(\boldsymbol{\Omega_1}) & Y_{10}^e(\boldsymbol{\Omega_1}) & Y_{11}^o(\boldsymbol{\Omega_1}) & Y_{11}^e(\boldsymbol{\Omega_1}) & Y_{20}^e(\boldsymbol{\Omega_1}) & \dots & Y_{99}^o(\boldsymbol{\Omega_1}) & Y_{99}^e(\boldsymbol{\Omega_1}) \\ Y_{00}^e(\boldsymbol{\Omega_2}) & Y_{10}^e(\boldsymbol{\Omega_2}) & Y_{11}^o(\boldsymbol{\Omega_2}) & Y_{11}^e(\boldsymbol{\Omega_2}) & Y_{20}^e(\boldsymbol{\Omega_2}) & \dots & Y_{99}^o(\boldsymbol{\Omega_2}) & Y_{99}^e(\boldsymbol{\Omega_2}) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ Y_{00}^e(\boldsymbol{\Omega_8}) & Y_{10}^e(\boldsymbol{\Omega_8}) & Y_{11}^o(\boldsymbol{\Omega_8}) & Y_{11}^e(\boldsymbol{\Omega_8}) & Y_{20}^e(\boldsymbol{\Omega_8}) & \dots & Y_{99}^o(\boldsymbol{\Omega_8}) & Y_{99}^e(\boldsymbol{\Omega_8}) \end{bmatrix} \text{ and}$$

$$\boldsymbol{M} = \begin{bmatrix} [\boldsymbol{M}] & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & [\boldsymbol{M}] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & [\boldsymbol{M}] \end{bmatrix}$$

(Please note that **0** represents a matrix of zeros of the appropriate dimension (as [M]))

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

$$[\boldsymbol{S}]_{\mathbf{12}} = \begin{bmatrix} \Sigma_{s0}^{1\to2} & 0 & \dots & 0 \\ 0 & \Sigma_{s1}^{1\to2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \Sigma_{s,9}^{1\to2} \end{bmatrix}$$

$\psi = ([\psi]_1\ [\psi]_2\ [\psi]_3)^T$ with

$[\psi]_1 = (\psi_1^1\ \psi_2^1 \dots \psi_8^1)^T$

$[\phi]_1 = (\phi_{00}^1\ \phi_{10}^1\ \theta_{11}^1\ \phi_{11}^1 \ldots \theta_{99}^1\ \phi_{99}^1)^T$

c)

$\boldsymbol{D} = \boldsymbol{M^T W}$ is the discrete-to-moment operator, with ***M*** defined earlier and ***W*** being a (8 x 8) diagonal matrix of diagonal matrices of quadrature weights.

d)

We do not need to form L in order to quantify our output vectors (fluxes and angular fluxes). Indeed, in the solving strategy, we are only interested to the action of a product of matrices including **L** on a vector.

Because of that, we can avoid forming L, which is computationally expensive, and speed up the calculation.

e)

- $\boldsymbol{L}\psi = \boldsymbol{MS}\phi + \boldsymbol{M}Q$
- $\phi = \boldsymbol{D}\psi \quad \rightarrow \quad \psi = \boldsymbol{D}^{-1}\phi$
- Inserting in (1): $\boldsymbol{L}(\boldsymbol{D}^{-1}\phi) = \boldsymbol{MS}\phi + \boldsymbol{M}Q$
- Define $b = \boldsymbol{DL}^{-1}\boldsymbol{M}Q$ and therefore multiply the previous equation by $\boldsymbol{DL}^{-1}$ from left
- $\phi = \boldsymbol{DL}^{-1}\boldsymbol{MS}\phi + b \quad \rightarrow \quad b = \phi - \boldsymbol{DL}^{-1}\boldsymbol{MS}\phi$
- $(\boldsymbol{1} - \boldsymbol{DL}^{-1}\boldsymbol{MS})\phi = b$ Note: Here ***1*** is the identity matrix
- Call $\boldsymbol{A} = (\boldsymbol{1} - \boldsymbol{DL}^{-1}\boldsymbol{MS})$ and solve the system of the type $\boldsymbol{A}x = b$