0.1 Diffusion Synthetic Acceleration

To accelerate source iteration in the LO system, a version of WLA DSA is used. The following derivations are to solve a diffusion equation which can be used to compute the source iteration error in the LO sweeps.

0.1.1 Forming a Continuous Diffusion Equation

Beginning with the P_1 equations for a steady-state problem

$$\frac{\partial J}{\partial x} + \sigma_a \phi = Q \tag{1}$$

$$\sigma_t J + \frac{1}{3}\frac{\partial \phi}{\partial x} = 0 \tag{2}$$

$$\tag{3}$$

spatial finite element moments are taken. The spatial moments are defined as

$$\langle \cdot \rangle_L = \frac{2}{h_i}\int_{x_{i-1/2}}^{x_{i+1/2}} \mathrm{d}x \, b_{L,i}(x) \, (\cdot) \tag{4}$$

$$\langle \cdot \rangle_R = \frac{2}{h_i}\int_{x_{i-1/2}}^{x_{i+1/2}} \mathrm{d}x \, b_{R,i}(x) \, (\cdot) \, . \tag{5}$$

where $b_{L,i}(x) = (x_{i+1/2} - x)/h_i$ and $b_{R,i}(x) = (x - x_{i-1/2})/h_i$. The scalar flux ϕ will ultimately be assumed continuous. For now it assumed LD, i.e., $\phi(x) = \phi_L b_L(x) + \phi_R b_R(x)$, for $x \in (x_{i-1/2}, x_{i+1/2})$. Taking the left moment, evaluating integrals, and rearranging yields

$$J_i - J_{i-1/2} + \frac{\sigma_{a,i} h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q \rangle_{L,i} \ , \tag{6}$$

where J_i is the average of the current over the cell. The moments of q are not simplified to be compatible with the LO moment equations. For the R moment

$$J_{i+1/2} - J_i + \frac{\sigma_{a,i} h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q \rangle_{R,i} \ . \tag{7}$$

The equation for the L moment is evaluated for cell $i+1$ and added to the R moment equation evaluated at i. The current is assumed continuous at

$i+1/2$ to eliminate the face current from the system. The sum of the two equations becomes

$$J_{i+1} - J_i + \frac{\sigma_{a,i+1}h_{i+1}}{2}\left(\frac{2}{3}\phi_{L,i+1} + \frac{1}{3}\phi_{R,i+1}\right) + \frac{\sigma_{a,i}h_i}{2}\left(\frac{1}{3}\phi_{L,i} + \frac{2}{3}\phi_{R,i}\right) = \frac{h}{2}\left(\langle q\rangle_{L,i+1} + \langle q\rangle_{R,i}\right). \quad (8)$$

The scalar flux is assumed continuous at each face, i.e., $\phi_{L,i+1} = \phi_{R,i} \equiv \phi_{i+1/2}$. We then approximate the cell-averaged currents with Fick's law as

$$J_i = -D_i\frac{\phi_{i+1/2} - \phi_{i-1/2}}{h_i}. \quad (9)$$

Combining the definition and rearranging yields the following discrete diffusion equation:

$$\left(\frac{\sigma_{a,i+1}h_{i+1}}{6} - \frac{D_{i+1}}{h_{i+1}}\right)\phi_{i+3/2} + \left(\frac{D_{i+1}}{h_{i+1}} + \frac{D_i}{h_i} + \frac{\sigma_{a,i+1}h_{i+1}}{3} + \frac{\sigma_{a,i}h_i}{3}\right)\phi_{i+1/2} + \left(\frac{\sigma_{a,i}h_i}{6} - \frac{D_i}{h_i}\right)\phi_{i-1/2} = \frac{h_{i+1}}{2}\langle q\rangle_{L,i+1} + \frac{h_i}{2}\langle q\rangle_{R,i} \ . \quad (10)$$

This system can be solved to get ϕ at each face.

Boundary Conditions

The LO system exactly satisfies the inflow boundary conditions, therefore we choose a vacuum boundary condition for the left-most cell. The equation for the left moment at the first cell is given by

$$J_1 - J_{1/2} + \frac{\sigma_{a,i}h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{L,i} \ , \quad (11)$$

The Marshak boundary condition for the vacuum inflow at face $x_{1/2}$ is given as

$$J^+_{1/2} = 0 = \frac{\phi_{1/2}}{4} + \frac{J_{1/2}}{2}, \quad (12)$$

which can be solved for $J_{1/2}$. Substitution of the above equation and Eq. (9) into Eq. (11) gives

$$\left(\frac{1}{2} + \frac{\sigma_{a,1}h_1}{3} - \frac{D_1}{h_1}\right)\phi_{1/2} + \left(\frac{\sigma_{a,1}h_1}{6} - \frac{D_1}{h_1}\right)\phi_{3/2} = \frac{h_i}{2}\langle q\rangle_{L,1} \quad (13)$$

a similar expression can be derived for the last cell.

0.1.2 Mapping Solution onto LD Unknowns

Solution of the continuous diffusion equation in the previous section provides correction values for ϕ on the faces, denoted as $\phi^C_{i+1/2}$. We now need to determine the correction these results provide for the LD representation of ϕ. To do this, first we take the L and R finite element moments of the P_1 equations. A LDFE dependence is assumed on the interior of the cell for J and ϕ. Taking moments of Eq. (1) and simplifying yields

$$J_{i+1/2} - \frac{J_{L,i} + J_{R,i}}{2} + \frac{\sigma_{a,i} h_i}{2}\left(\frac{1}{3}\phi_{L,i} + \frac{2}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q \rangle_{R,i} \tag{14}$$

$$\frac{J_{L,i} + J_{R,i}}{2} - J_{i-1/2} + \frac{\sigma_{a,i} h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q \rangle_{L,i} \tag{15}$$

The moment equations for Eq. (2) are

$$\frac{1}{3}\left(\phi_{i+1/2} - \frac{\phi_{i,L} + \phi_{i,R}}{2}\right) + \frac{\sigma_{t,i} h_i}{2}\left(\frac{1}{3}J_{L,i} + \frac{2}{3}J_{R,i}\right) = 0 \tag{16}$$

$$\frac{1}{3}\left(\frac{\phi_{i,L} + \phi_{i,R}}{2} - \phi_{i-1/2}\right) + \frac{\sigma_{t,i} h_i}{2}\left(\frac{2}{3}J_{L,i} + \frac{1}{3}J_{R,i}\right) = 0 \tag{17}$$

The currents and fluxes on faces are decomposed into half-range values. This allows the cells to be decoupled by using values of $\phi^C_{i+1/2}$.

First, the definitions at face $x_{i+1/2}$ are considered. The current is composed as $J_{i+1/2} = J^+_{i+1/2} - J^-_{i+1/2}$ and the scalar flux as $\phi_{i+1/2} = \phi^+_{i+1/2} + \phi^-_{i+1/2}$, where $+$ and $-$ denote the positive and negative half ranges of μ, respectively. The negative direction values $J^-_{i+1/2}$ and $\phi^-_{i+1/2}$ are upwinded from cell $i+1$. However, we approximate these values based on $\phi^C_{i+1/2}$. The incoming flux is assumed isotropic, which yields an incoming current of $J^-_{i+1/2} = \gamma\frac{\phi^C_{i+1/2}}{2}$, where γ accounts for the different between the LO equations estimate of the current compared to the P_1 assumption of the flux that is used in the approximate equations. Similarly, the half-range flux on the face is $\phi^-_{i+1/2} = \frac{\phi^-_{i+1/2}}{2}$. In the positive direction, at the right face, the values of ϕ and J are based on the LD representation within the cell at that face, i.e., $\phi_{R,i}$ and $J_{R,i}$. The standard P_1 approximation for the half-range currents and fluxes are used[?], i.e.,

$$J^{\pm} = \frac{\gamma\phi}{2} \pm \frac{J}{2} \tag{18}$$

$$\phi\pm = \frac{\phi}{2} \pm \frac{3J\gamma}{2}. \tag{19}$$

Thus, for the right face and positive half-range,

$$J^{+}_{i+1/2} = \frac{\gamma}{2}\phi_{i,R} + \frac{J_{i,R}}{2} \tag{20}$$

$$\phi^{+}_{i+1/2} = \frac{\phi_{i,R}}{2} + \frac{3\gamma}{2}J_{i,R} \tag{21}$$

The currents and partial fluxes are defined similarly for $x_{i-1/2}$. Combining these results, the remaining equations necessary for solving the system are

$$J_{i+1/2} = \frac{\gamma}{2}\phi_{i,R} + \frac{J_{i,R}}{2} - \frac{\gamma}{2}\phi^{C}_{i+1/2} \tag{22}$$

$$J_{i-1/2} = \frac{\gamma}{2}\phi^{C}_{i-1/2} - \left(\frac{\gamma}{2}\phi_{i,L} - \frac{J_{i,L}}{2}\right) \tag{23}$$

$$\phi_{i+1/2} = \frac{1}{2}\phi_{i,R} + \frac{3\gamma J_{i,R}}{2} + \frac{1}{2}\phi^{C}_{i+1/2} \tag{24}$$

$$\phi_{i-1/2} = \frac{1}{2}\phi_{i,L} - \frac{3\gamma J_{i,L}}{2} + \frac{1}{2}\phi^{C}_{i-1/2} \tag{25}$$

These equations are substituted back into the original system to produce

$$\frac{\gamma}{2}\phi_{i,R} + \frac{J_{i,R}}{2} - \frac{\gamma}{2}\phi^{C}_{i+1/2} - \frac{J_{L,i} + J_{R,i}}{2} + \frac{\sigma_{a,i}h_i}{2}\left(\frac{1}{3}\phi_{L,i} + \frac{2}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{R,i} \tag{26}$$

$$\frac{J_{L,i} + J_{R,i}}{2} - \left(\frac{\gamma}{2}\phi^{C}_{i-1/2} - \frac{\gamma}{2}\phi_{i,L} + \frac{J_{i,L}}{2}\right) + \frac{\sigma_{a,i}h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{L,i} \tag{27}$$

$$\frac{1}{3}\left(\frac{1}{2}\phi_{i,R} + \frac{3\gamma J_{i,R}}{2} + \frac{1}{2}\phi^{C}_{i+1/2} - \frac{\phi_{i,L} + \phi_{i,R}}{2}\right) + \frac{\sigma_{t,i}h_i}{2}\left(\frac{1}{3}J_{L,i} + \frac{2}{3}J_{R,i}\right) = 0 \tag{28}$$

$$\frac{1}{3}\left(\frac{\phi_{i,L} + \phi_{i,R}}{2} - \left[\frac{1}{2}\phi_{i,L} - \frac{3\gamma J_{i,L}}{2} + \frac{1}{2}\phi^{C}_{i-1/2}\right]\right) + \frac{\sigma_{t,i}h_i}{2}\left(\frac{2}{3}J_{L,i} + \frac{1}{3}J_{R,i}\right) = 0 \tag{29}$$

These equations are completely local to each cell and fully defined. The system can be solved for the the desired unknowns $\phi_{i,L}$, $\phi_{i,R}$, $J_{i,L}$, and $J_{i,R}$.

0.1.3 Alternative update equations

As an alternative approach, we can use the following equation (which is true for P_1 expansion of the flux) to eliminate the incoming currents:

$$\phi = 2(J^+ + J^-) \tag{30}$$

At a face, the continuous solution provides ϕ, and the current are eliminated in terms of the outflow current on that face. For the left face, the total current then becomes

$$J_{i-1/2} = J^+_{i-1/2} - J^-_{i-1/2} = \frac{\phi}{2} - 2J^-_{i-1/2} \tag{31}$$

Substituting the continuous solution, the current becomes

$$J_{i-1/2} = \frac{\phi^C_{i-1/2}}{2} - 2J^-_{i-1/2} = \frac{\phi^C_{i-1/2}}{2} - 2\left(\frac{\gamma}{2}\phi_{i,L} - \frac{J_{i,L}}{2}\right) \tag{32}$$

Using similar equation for all the inflow currents, the balance equations for ϕ become

$$\left(\gamma\phi_{i,R} + J_{i,R} - \frac{\phi^C_{i+1/2}}{2}\right) - \frac{J_{L,i} + J_{R,i}}{2} + \frac{\sigma_{a,i}h_i}{2}\left(\frac{1}{3}\phi_{L,i} + \frac{2}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{R,i} \tag{33}$$

$$\frac{J_{L,i} + J_{R,i}}{2} - \left(\frac{\phi^C_{i-1/2}}{2} - \gamma\phi_{i,L} + J_{i,L}\right) + \frac{\sigma_{a,i}h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{L,i} \tag{34}$$

We can also break up ϕ in Eq. (31) into its half-range components, producing the equations

$$\left(\gamma\phi_{i,R} + J_{i,R} - \left[\gamma\frac{\phi^C_{i+1/2}}{2} + \frac{\phi_{i,R}}{4} + \frac{3}{4}\gamma J_{i,R}\right]\right) - \frac{J_{L,i} + J_{R,i}}{2} + \frac{\sigma_{a,i}h_i}{2}\left(\frac{1}{3}\phi_{L,i} + \frac{2}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{R,i} \tag{35}$$

$$\frac{J_{L,i} + J_{R,i}}{2} - \left(\left[\frac{\gamma}{2}\phi^C_{i-1/2} + \frac{\phi_{i,L}}{4} - \frac{3}{4}\gamma J_{i,L}\right] - \gamma\phi_{i,L} + J_{i,L}\right) + \frac{\sigma_{a,i}h_i}{2}\left(\frac{2}{3}\phi_{L,i} + \frac{1}{3}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{L,i} \tag{36}$$

0.1.4 DSA Source Definition

The above discretization procedure is used to determine the error in the scalar flux. The sources $\langle q \rangle_{L/R}$ thus need to be defined. They are simply the residual in the scattering iterations, given by

$$q = \sigma_s \left(\phi^{l+1/2} - \phi^l \right). \tag{37}$$

The spatial moments are straight forward:

$$\langle q \rangle_{L,i} = \sigma_{s,i} \left(\langle \phi^{l+1/2} \rangle_{L,i} - \langle \phi^l \rangle_{L,i} \right) \tag{38}$$

0.1.5 Updating the LO Unkowns

We now have a correction to J and ϕ for the volumetric finite element unknowns. Because we are interested in the time-dependent solution, we need to accelerate the solution for the half-range fluxes, rather than just the scalar flux. Beginning with the P_1 approximation for the angular intensity

$$\delta I(\mu) = \frac{\delta\phi}{4\pi} + \frac{3\delta J}{4\pi}\mu. \tag{39}$$

Taking the half range integrals gives

$$\delta\phi^{\pm} = \frac{\delta\phi}{2} \pm \frac{3\delta J}{4} \tag{40}$$

Thus, each of the volumetric moments can be updated accordingly.