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 at faces. The scalar flux is assumed linear on the interior of the cell, 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. To allow for the use of lumped or standard LD in these equations, we introduce the factor θ, with $\theta = 1/3$ for standard LD, and $\theta = 1$ for lumped LD. The diffusion equation becomes

$$\left(\frac{\sigma_{a,i+1} h_{i+1}}{4} (1-\theta) - \frac{D_{i+1}}{h_{i+1}} \right) \phi_{i+3/2} + \left(\frac{D_{i+1}}{h_{i+1}} + \frac{D_i}{h_i} + \left(\frac{1+\theta}{2} \right) \left[\frac{\sigma_{a,i+1} h_{i+1}}{2} + \frac{\sigma_{a,i} h_i}{2} \right] \right) \phi_{i+1/2} + \left(\frac{\sigma_{a,i} h_i}{4} (1-\theta) - \frac{D_i}{h_i} \right) \phi_{i-1/2} = \frac{h_{i+1}}{2} \langle q \rangle_{L,i+1} + \frac{h_i}{2} \langle q \rangle_{R,i} \ . \quad (11)$$

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

$$J_1 - J_{1/2} + \frac{\sigma_{a,i} h_i}{2} \left(\frac{1+\theta}{2} \phi_{L,i} + \frac{1-\theta}{2} \phi_{R,i} \right) = \frac{h_i}{2} \langle q \rangle_{L,i} \ , \quad (12)$$

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

$$J^+_{1/2} = 0 = \frac{\phi_{1/2}}{4} + \frac{J_{1/2}}{2}, \tag{13}$$

which can be solved for $J_{1/2}$. Substitution of the above equation and Eq. (9) into Eq. (12) gives

$$\left(\frac{1}{2} + \sigma_{a,1} h_1 \frac{1+\theta}{4} - \frac{D_1}{h_1}\right)\phi_{1/2} + \left(\sigma_{a,1} h_1 \frac{1-\theta}{4} - \frac{D_1}{h_1}\right)\phi_{3/2} = \frac{h_i}{2}\langle q\rangle_{L,1} \tag{14}$$

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

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

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

The moment equations for Eq. (2) are

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

$$\frac{1}{3}\left(\frac{\phi_{i,L} + \phi_{i,R}}{2} - \phi_{i-1/2}\right) + \frac{\sigma_{t,i} h_i}{2}\left(\frac{2}{3}J_{L,i} + \frac{1}{3}J_{R,i}\right) = 0 \tag{18}$$

Using similar equation for all the inflow currents, the balance equations for ϕ become The face terms $J_{i\pm1/2}$ and $\phi_{i\pm1/2}$ need to be eliminated from the system. The scalar flux is assumed to be the value provided by the continuous diffusion solution at each face, i.e., $\phi_{i\pm1/2} = \phi^C_{i\pm1/2}$. The currents are decomposed into half-range values to decouple the equations between cells. At $x_{i+1/2}$, the current is composed as $J_{i+1/2} = J^+_{i+1/2} - J^-_{i+1/2}$, where

$+$ and $-$ denote the positive and negative half ranges of μ, respectively. Typically, the incoming current $J^-_{i+1/2}$ is upwinded from cell $i+1$. However, we approximate the incoming current based on $\phi^C_{i+1/2}$. The P_1 approximation provides the following relation

$$\phi = 2(J^+ + J^-). \tag{19}$$

At $x_{i+1/2}$, the above expression is solved for the incoming current $J^-_{i+1/2}$. The total current becomes, with $\phi_{i+1/2} = \phi^C_{i+1/2}$,

$$J_{i+1/2} = J^+_{i+1/2} - J^-_{i+1/2} = 2J^+_{i+1/2} - \frac{\phi^C_{i+1/2}}{2}, \tag{20}$$

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.,

$$J^{\pm} = \frac{\gamma\phi}{2} \pm \frac{J}{2}, \tag{21}$$

where γ accounts for the difference between the LO parameters and the true P_1 approximation. Thus, for the right face and positive half-range,

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

A similar expression can be derived for $x_{i-1/2}$. The total currents at each face are thus

$$J_{i+1/2} = \gamma\phi_{i,R} + J_{i,R} - \frac{\phi^C_{i+1/2}}{2} \tag{23}$$

$$J_{i-1/2} = \frac{\phi^C_{i-1/2}}{2} - \gamma\phi_{i,L} + J_{i,L} \tag{24}$$

Substitution of these results back into the LD balance equations and introduction of the lumping notation yields the final equations

$$\left(\gamma\phi_{i,R} + J_{i,R} - \frac{\phi^C_{i+1/2}}{2}\right) - \frac{J_{L,i}+J_{R,i}}{2} + \frac{\sigma_{a,i}h_i}{2}\left(\frac{(1-\theta)}{2}\phi_{L,i} + \frac{(1+\theta)}{2}\phi_{R,i}\right) = \frac{h_i}{2}\langle q\rangle_{R,i} \tag{25}$$

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

$$\frac{1}{3}\left(\phi^C_{i+1/2} - \frac{\phi_{i,L}+\phi_{i,R}}{2}\right) + \frac{\sigma_{t,i}h_i}{2}\left(\frac{(1-\theta)}{2}J_{L,i} + \frac{(1+\theta)}{2}J_{R,i}\right) = 0 \tag{27}$$

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

The above 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 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

$$q = \sigma_s\left(\phi^{l+1/2} - \phi^l\right). \tag{29}$$

The spatial moments are straight forward:

$$\langle q\rangle_{L,i} = \sigma_{s,i}\left(\langle\phi^{l+1/2}\rangle_{L,i} - \langle\phi^l\rangle_{L,i}\right) \tag{30}$$

The above equation is valid for lumping or standard LD. This is because the LO moments are defined differently for LLD or LD, resulting in equations that are consistent. For instance, for lumped LD, the LO system uses the spatial closure that the edge value is defined as the moment, i.e., $\langle\phi\rangle_{R,i} \equiv \phi_{R,i}$. For a standard lumped source, we desire the right equation to have $\langle q\rangle_{R,i} = \sigma_s(\phi^{l+1/2}_{R,i} - \phi^l_{R,i})$. Substituting the lumped closure into the right hand side of this equation gives back the original equation, i.e., $\langle q\rangle_{R,i} = \sigma_{s,i}\left(\langle\phi^{l+1/2}\rangle_{R,i} - \langle\phi^l\rangle_{R,i}\right)$. The same is true for standard LD.

0.1.4 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. We only accelerate the zeroth moment of the angular intensity. The error in the scalar intensities are defined as

$$\delta\phi^{\pm} = \frac{\delta\phi}{2} \pm \frac{3\delta J}{4} \tag{31}$$

Spatial moments are taken of $\delta\phi^{\pm}$, using the lumping notation of LD on the interior

$$\langle\delta\phi^{\pm}\rangle_L = \frac{1+\theta}{2}\delta\phi^{\pm}_L + \frac{1-\theta}{2}\delta\phi^{\pm}_R \tag{32}$$

$$\langle\delta\phi^{\pm}\rangle_R = \frac{1-\theta}{2}\delta\phi^{\pm}_L + \frac{1+\theta}{2}\delta\phi^{\pm}_R, \tag{33}$$

where Eq. (31) can be used to get in terms of $\delta\phi_{L/R}$ and $\delta J_{L/R}$. It is noted that for consistency, the updates to the moments depend on the lumping notation, even though the sources are defined the same in both cases.

0.2 Analytic Neutronics answer for Source fixup

In this section we model a fixed-source, pure-absorber neutronics calculation where we know the analytic answer to test our fixup. If we make the mesh thick enough, we can set the solution to be the equilibrium answer $\psi(x) = \frac{q(x)}{2\sigma_a}$. For a general isotropic source $Q(x)$, the 1D transport equation to be solved is

$$\mu\frac{\partial\psi}{\partial x} + \sigma_a\psi(x,\mu) = \frac{q(x)}{2} \tag{34}$$

with boundary condition $\psi(0,\mu) = \psi_{inc}$, $\mu > 0$ and $\psi(x_R,\mu) = \frac{q(x_R)}{2\sigma_a}$ for $\mu < 0$, where x_R is the right boundary. This first order differential equation is solved using an integration factor. The solution to this equation for $\mu > 0$ is given by

$$\psi(x,\mu) = \psi_{inc}e^{\frac{-\sigma_a x}{\mu}} + \int_0^x \frac{q(x')}{2\mu}e^{\frac{-\sigma_a x'}{\mu}}\mathrm{d}x', \quad \mu > 0 \tag{35}$$

Integration of this result over the positive half range of μ gives

$$\phi^{+}(x) = \psi_{inc}\,\mathrm{E}_2(\sigma_a x) + \frac{1}{2}\int_0^x q(x')\,\mathrm{E}_1(\sigma_a x')\mathrm{d}x'. \tag{36}$$

In the simplification of a constant source, the integral reduces to

$$\phi^{+}(x) = \psi_{inc}\,\mathrm{E}_2(\sigma_a x) + \frac{q}{2\sigma_a}\left(1 - \mathrm{E}_2(\sigma_a x)\right). \tag{37}$$

Also, for a constant source the solution for the negative half range becomes a constant, i.e.,

$$\phi^{-}(x) = \frac{q}{\sigma_a} \tag{38}$$

Combination of the above two equations gives the solution for the scalar flux:

$$\phi(x) = \psi_{inc}\,\mathrm{E}_2(\sigma_a x) + \frac{q}{2\sigma_a}\left(1 - \mathrm{E}_2(\sigma_a x)\right) + \frac{q}{\sigma_a}. \tag{39}$$

0.2.1 MC solution with LDD trial space

The inclusion of the outflow discontinuity has a minimal effect on the treatment of the residual source. The residual source and process of estimating moments of the error on the interior of a space-angle cell is unchanged. The process of estimating the solution on the outgoing face requires tallying the solution when particles leave a cell. The specific tallies are described in Section **??**. As far as face source of the residual, there is no need to change the residual source on faces either, however care must be taken in how the error is added to the solution on a frace.

To demonstrate that the residual face source is unchanged, it is necessary to look at the δ-function face source, which results from the discontinuity in the trial space. For positive flow, at the node $x_{i+1/2}$, the face source is defined as

$$r_{\text{face}} = -\mu\frac{\partial I^{(m)}}{\partial x}\Big|_{x_{i+1/2}} \tag{40}$$

PROOF THAT FACE SOURCES CANCEL OUT IN EFFECT AND THAT SOURCES CANCEL OUT

0.2.2 Face Tallies and correction near $\mu = 0$

Face-averaged estimators of the angular error are required to compute the outflow for estimating the spatial closure. The standard face-based estimators [?, ?] are used. The tallies are weighted by the appropriate basis functions to compute a linear projection along the face. The tally score, for the angular-average error on a face, is defined as

$$\hat{\epsilon}_{a,i\pm 1/2,j} = \frac{1}{N} \sum_{m=1}^{N_{i+1/2,j}} \frac{w_m(x_{i\pm 1/2}, \mu)}{h|\mu|} \tag{41}$$

where N is the number of histories performed and $N_{i+1/2,j}$ is the number of histories that crossed the surface of interest, in the appropriate angular bin. For the first moment, the tally is

$$\hat{\epsilon}_{\mu,i\pm 1/2,j} = \frac{1}{N} \sum_{m=1}^{N_{i+1/2,j}} 6 \frac{\mu - \mu_j}{h_\mu} \frac{w_m(x_{i\pm 1/2}, \mu)}{|\mu|} \tag{42}$$

Near $\mu = 0$, particles can contribute large scores which can lead to large and unbounded variance [?]. To avoid this, the standard fixup is used [?, ?]. If $|\mu|$ is below some small cutoff μ_{cut}, then particles contribute the average score over the range $(0, \mu_{cut})$, based on an approximate isotropic intensity. Assuming an isotropic intensity, the average of $1/|mu|$ is given by

$$\tag{43}$$