6.5 Source Iteration

The diamond difference equations we have defined give us a system of $I \times J \times K \times N_{\text{angles}}$ unknowns for a single-group problem. For 3-D problems the number of angles can easily be in the hundreds or thousands. This makes the system be solved much larger than an equivalent diffusion problem. Fortunately, we can solve discrete ordinates problems without storing the angular fluxes through an approach known as *source iteration*.

To develop source iteration in 1-D slabs we write Eq. (6.27) using the iteration index ℓ where we evaluate the moments and sources at level ℓ and the angular fluxes on the left-hand side at $\ell + 1$:

(6.29)

The way this works, we begin with $\phi_{li}^{\ell+1} = 0$. We then calculate ψ_{1i} from Eqs. (6.29) and (6.24). We update the moments as

$$\phi_{li}^{\ell+1} := \phi_{li}^{\ell+1} + w_1 P_l(\mu_1) \frac{2l+1}{2} \Sigma_{\text{s}l}(z) \psi_{1i}, \tag{6.30}$$

and then, for $n = 2, \ldots, N$, we compute ψ_{ni} and update

$$\phi_{li}^{\ell+1} := \phi_{li}^{\ell+1} + w_n P_l(\mu_n) \frac{2l+1}{2} \Sigma_{\text{s}l}(z) \psi_{ni}. \tag{6.31}$$

This approach is beneficial for two main reasons. The first is that we never have to store the entire angular flux. The second is that solving for a single ordinate is a known as a lower-triangular solve. To see this we look at the equations for $\mu > 0$ beginning at $i = 1$:

$$\mu_n \frac{\psi_{n,3/2}^{\ell+1}}{h_z} + \frac{\Sigma_{\text{t}1}}{2} \psi_{n,3/2}^{\ell+1} = \sum_{l=0}^{L} \frac{2l+1}{2} P_l(\mu_n) \Sigma_{\text{s}l1} \phi_{l1}^{\ell} + q_{n1} + \quad . \tag{6.32}$$

Note this is an equation only for $\psi_{n,3/2}^{\ell+1}$. We can solve it, and then compute a contribution to ϕ_{l1}. The next equation is the $i = 2$ equation:

$$\mu_n \frac{\psi_{n,5/2}^{\ell+1}}{h_z} + \frac{\Sigma_{\text{t}2}}{2} \psi_{n,5/2}^{\ell+1} = \sum_{l=0}^{L} \frac{2l+1}{2} P_l(\mu_n) \Sigma_{\text{s}l2} \phi_{l2}^{\ell} + q_{n2} + \quad . \tag{6.33}$$

We can solve for $\psi_{n,5/2}^{\ell+1}$ because we already know $\psi_{n,3/2}^{\ell+1}$. This also allows us to calculate a contribution to ϕ_{l2} as in Eq. (6.31). This continues until the last

equation when we get $\psi^{\ell+1}_{n,I+5/2}$ from

$$\mu_n \frac{\psi^{\ell+1}_{n,I+1/2}}{h_z} + \frac{\Sigma_{\mathrm{t}I}}{2}\psi^{\ell+1}_{n,I+1/2} = \sum_{l=0}^{L} \frac{2l+1}{2} P_l(\mu_n)\Sigma_{\mathrm{s}lI}\phi^{\ell}_{lI} + q_{nI} + \quad , \tag{6.34}$$

to allow us to calculate a contribution from angle μ_n to $\phi^{\ell+1}_{lI}$. For ordinates where $\mu_n < 0$, we go the other way. We start at edge $I - 1/2$ to compute

$$-\mu_n \frac{\psi^{\ell+1}_{n,I-1/2}}{h_z} + \frac{\Sigma_{\mathrm{t}I}}{2}\psi^{\ell+1}_{n,I-1/2} = \sum_{l=0}^{L} \frac{2l+1}{2} P_l(\mu_n)\Sigma_{\mathrm{s}lI}\phi^{\ell}_{lI} + q_{nI} - \quad . \tag{6.35}$$

This continues moving right to left until we reach the left boundary:

$$-\mu_n \frac{\psi^{\ell+1}_{n,1/2}}{h_z} + \frac{\Sigma_{\mathrm{t}1}}{2}\psi^{\ell+1}_{n,1/2} = \sum_{l=0}^{L} \frac{2l+1}{2} P_l(\mu_n)\Sigma_{\mathrm{s}l1}\phi^{\ell}_{l1} + q_{n1} - \quad . \tag{6.36}$$

In summary for ordinates with $\mu_n > 0$ we start at the left edge of the system and "sweep" through the mesh to the right boundary, updating the moments at iteration $\ell + 1$ along the way. When $\mu_n < 0$, we go the opposite direction: from right to left. The traversal of the mesh to compute the new values of the angular flux is known as a transport sweep.

The source iteration procedure extends to multiple dimensions. In 2-D we start at one of the corners of the mesh and sweep toward the other corner. For example, if $\mu_n > 0$, and $\eta_n > 0$, we would start at zone $i = 1$ and $j = 1$, and then we could finish the remaining cells in the x direction at $j = 1$, sweeping from left to right. Then we can go to $j = 2$ and complete all the zones in the x direction. This continues until $j = J$. This procedure changes to begin in a different corner depending on the signs of μ_n and η_n.

In 3-D we still start at one of 8 corners and update planes at a time. To extend the example from above if μ_n, η_n, ξ_N are positive, the we would start at $i = j = k = 1$. After updating that zone, we can then update all other i's with $j = k = 1$. We then update all i's with $j = 2$ and $k = 1$ before proceeding to $j = 3$ and $k = 1$ and so on until we solve all i's with $j = J$ and $k = 1$. At that point we increment to $k = 2$ and do the same thing.

The procedure for performing the sweep in 3-D is given in Algorithm 3.

```
Data: Cross sections, previous iteration moments, and incoming angular
      fluxes on boundaries
Result: Updated moments
for n ∈ [0, N_angles] do
    if μ_n > 0 then
        Zstart = 1;
        Zend = K;
    end
    else
        Zstart = K;
        Zend = 1;
    end
    if ξ_n > 0 then
        Ystart = 1;
        Yend = J;
    end
    else
        Ystart = J;
        Yend = 1;
    end
    if η_n > 0 then
        Xstart = 1;
        Xend = I;
    end
    else
        Ystart = I;
        Yend = 1;
    end
    for i ∈[XStart,XEnd] do
        for j ∈[YStart,YEnd] do
            for k ∈[ZStart,ZEnd] do
                Update ψ_n in zone and compute contribution to the
                moments in zone ijk.
            end
        end
    end
end
```

Algorithm 3: For performing a transport sweep in 3-D on a Cartesian grid.

The source iteration can converge slowly for problems where there is little absorption and net leakage out of the boundary. To see why this is, we look at the transport equation in 1-D for an infinite, homogeneous medium with

isotropic scattering and sources updated via source iteration

(6.37)

If we define the error in the iteration to be

$$f^{(\ell)}(z,\mu) = \psi(z,\mu) - \psi^{(\ell)}(z,\mu), \qquad g^{(\ell)}(z) = \int_{-1}^{1} d\mu\, f^{(\ell)}(z,\mu),$$

we can rewrite this equation as

$$\left(\mu_n \frac{\partial}{\partial z} + \Sigma_{\rm t}\right) f_n^{(\ell+1)}(z) = \frac{\Sigma_{\rm s}}{2} g^{(\ell)}. \tag{6.38}$$

We next Fourier transform the spatial variable to get

(6.39)

The next step is to solve this equation for the $\hat{f}_n^{(\ell+1)}$ to get

(6.40)

Integrating this equation over μ leads to a relation for the error in the scalar flux for iteration $\ell + 1$ as a function of the error at ℓ as

Note that

The error in the angular flux at iteration $\ell + 1$ is then

(6.42)

Finally, we perform the inverse Fourier transform to get

(6.43)

This can be used to bound the error as

where B is a constant. The importance of Eq. (6.44) is that as Σ_s/Σ_t approaches 1, the iterations have their convergence slowed, or stopped completely.

Therefore, in an infinite medium made of a pure scatter, source iteration cannot be used to compute the solution. This does not seem seem like a strong restriction, yet in practice it can be quite limiting. When the scattering ratio is large and the amount of leakage from the system is small, the reduction in the error in the system can still be quite small for each iteration. This fact has spurred a great deal of research into accelerating source iteration. Algorithms such as diffusion synthetic acceleration (DSA) use an auxiliary diffusion calculation to help converge the scattering source, and have been widely used in the transport community. Unfortunately, most DSA schemes are less effective in heterogeneous media and they can be difficult to implement. We, instead, will cover two different approaches to accelerating transport calculations.

We can also think of source iteration as computing the solution as the sum of scalar fluxes of neutrons that have collided a given number of times. If the initial guess for the solution is zero everywhere, the angular fluxes from the first iteration are

That is the angular flux after the first iteration represents particles that have not had a collision, sometimes called the uncollided flux. The solution from the

second iteration is given by

This implies that $\psi^2 - \psi^1$ is the angular flux of particles that have collided exactly once or the first-collided flux. We can generalize this to get that $\psi^M - \psi^{M-1}$ is the Mth-collided flux. Clearly, if there is any absorption in the system $\psi^M - \psi^{M-1}$ goes to zero as $M \to \infty$. For a given convergence tolerance, we can estimate a worst case scenario for the number of iterations required to converge as

$$\text{iterations} \leq \log \tau \left[\log \sup_i \left(\frac{\Sigma_{si}}{\Sigma_{ti}} \right) \right]^{-1}, \tag{6.45}$$

where τ is the required difference between iterations.

6.6 GMRES

The generalized minimum residual (GMRES) method is an iterative method for solving linear systems of equations. The benefit of GMRES is that it only requires the action of a linear operator on a vector, and not the entire matrix. This means that we can compute the solution for the scalar flux (and other moments) for a problem without storing any angular flux solutions, as we did in source iteration. Furthermore, GMRES for a vector of unknowns of size N is guaranteed to converge to a solution in N iterations (in contrast to the stagnation of source iteration).

GMRES is known as a Krylov method because it builds what is known as the Krylov subspace with each iteration. For the linear system given by

$$\mathbf{A}\vec{x} = \vec{b}, \tag{6.46}$$

at the nth iteration it finds the best possible solution that lives in the Krylov subspace, K_n, defined by

(6.47)

The GMRES method augments the Krylov subspace at each iteration, and solves a least-squares problem of size n to find the vector in K_n that minimizes the residual. To accomplish an iteration the only place that the matrix $\mathbf{A}$ is needed is in multiplying a vector by $\mathbf{A}$.

For our purposes, we will derive a linear operator that acts like a matrix on the scalar flux. We start by writing source iteration using some operator notation. For this derivation our notation is for 1-D slabs. We then write an iteration of source iteration as

$$\mathbf{L}_n \vec{\psi}_n^{\ell+1} = \mathbf{MS}\vec{\phi}^{\ell} + \vec{q}_n, \tag{6.48}$$

where

$$\vec{\psi}_n^{\ell+1} = \begin{cases} \left(\psi_{n,3/2}^{\ell+1}, \ldots, \psi_{n,I+1/2}^{\ell+1}\right)^{\mathrm{t}} & \mu_n > 0 \\ \left(\psi_{n,1/2}^{\ell+1}, \ldots, \psi_{n,I-1/2}^{\ell+1}\right)^{\mathrm{t}} & \mu_n < 0 \end{cases}$$

$$\vec{q}_n = \begin{cases} \left(q_{n1} + \mu_n \frac{f(\mu_n)}{h_z} - \frac{\Sigma_{\mathrm{t}i}}{2} f(\mu_n), \ldots, q_{nI}\right)^{\mathrm{t}} & \mu_n > 0 \\ \left(q_{n1}, \ldots, q_{nI} - \mu_n \frac{f(\mu_n)}{h_z} - \frac{\Sigma_{\mathrm{t}i}}{2} f(\mu_n)\right)^{\mathrm{t}} & \mu_n < 0 \end{cases},$$

and

$$\vec{\phi} = (\phi_{01}, \phi_{11}, \ldots, \phi_{L1}, \phi_{02}, \ldots, \phi_{0I}, \ldots, \phi_{LI})^{\mathrm{t}}.$$

The $\mathbf{L}_n$ operator is the streaming and removal operator which for row i is

$$(\mathbf{L}_n \vec{\psi})_i = \mu_n \frac{\psi_{n,i+1/2} - \psi_{n,i-1/2}}{h_z} + \frac{\Sigma_{\mathrm{t}i}}{2} \left(\psi_{n,i+1/2} + \psi_{n,i-1/2}\right). \tag{6.49}$$

The structure of the matrix $\mathbf{L}$ for $\mu_n > 0$ is

$$\mathbf{L}_n = \begin{pmatrix} * & & & & \\ * & * & & & \\ 0 & * & * & & \\ \vdots & & \ddots & \ddots & \\ 0 & \ldots & 0 & * & * \end{pmatrix}, \quad \mu_n > 0. \tag{6.50}$$

This is a lower triangular matrix, hence the notation $\mathbf{L}_n$. For $\mu_n < 0$ the matrix is upper triangular (though we don't change the notation)

$$\mathbf{L}_n = \begin{pmatrix} * & * & 0 & \ldots & 0 \\ & \ddots & \ddots & & \vdots \\ & & * & * & 0 \\ & & & * & * \\ & & & & * \end{pmatrix}, \quad \mu_n < 0. \tag{6.51}$$

The *scattering* operator $\mathbf{S}$ computes the scattering given moments. This is a block diagonal matrix with elements where each spatial zone i has a block matrix given by

$$(\mathbf{S}\vec{\phi})_{mi} = \Sigma_{smi} \phi_{mi}. \tag{6.52}$$

The result of this operation is a vector with LI elements that is then operated on by the *moment to discrete* operator that takes moments and turns them into discrete ordinates values. For zone i this looks like

$$(\mathbf{M}\vec{\varphi})_i = \sum_{l=0}^{L} \frac{2l+1}{2} P_l(\mu_n) \varphi_{li}. \tag{6.53}$$

Looking at the solution procedure from this point of view indicates that we can compute the source iteration update using matrix vector products. To

proceed we define a *discrete to moment* operator that takes angular fluxes and computes moments. The discrete to moment operator is defined as

$$\mathbf{D}\vec{\Psi} = \left[\sum_{n=1}^{N} w_n P_0(\mu_n)\vec{\psi}_n, \sum_{n=1}^{N} w_n P_1(\mu_n)\vec{\psi}_n, \ldots, \sum_{n=1}^{N} w_n P_L(\mu_n)\vec{\psi}_n\right]^{\mathrm{t}} = \vec{\phi}, \tag{6.54}$$

where the vector $\vec{\Psi}$ is a vector of vectors of angular fluxes

(6.55)

$\vec{Q}$ is The discrete-to-moment operator takes the entire angular flux (a vector of length IN) and maps it to a vector of moments with length IL. We additionally define the $\mathbf{L}$ operator as

$$\mathbf{L}\vec{\Psi} = \left[\mathbf{L}_1\vec{\psi}_1, \ldots, \mathbf{L}_N\vec{\psi}_N\right]^{\mathrm{t}}. \tag{6.56}$$

Using these operators we can write $\vec{\Psi}$ as the solution to the linear system of equations

$$\left(\mathbf{L} - \mathbf{MSD}\right)\vec{\Psi} = \vec{Q}, \tag{6.57}$$

where $\vec{Q}$ is a vector of the sources $\vec{q}_n$. This form is useful, though we do not really need to know the entire angular flux. Rather, we want the L moments and typically $L \ll N$. We note that the operator $\mathbf{L}$ is a block diagonal operator where each block is either upper or lower triangular. This means that we can easily compute the action of $\mathbf{L}^{-1}$ on a vector. In fact, we can compute the action of $\mathbf{L}^{-1}$ on a vector by performing an iteration of source iteration where the source is the vector we want to apply $\mathbf{L}^{-1}$ to.

We operate on Eq. (6.57) by $\mathbf{L}^{-1}$ to get

$$\left(\mathbf{I} - \mathbf{L}^{-1}\mathbf{MSD}\right)\vec{\Psi} = \mathbf{L}^{-1}\vec{Q}. \tag{6.58}$$

Then, applying the moment to discrete operator we get a linear system just for the moments as

$$\left(\mathbf{I} - \mathbf{DL}^{-1}\mathbf{MS}\right)\vec{\phi} = \mathbf{DL}^{-1}\vec{Q}. \tag{6.59}$$

Therefore, we can solve for the moments of the discrete ordinates solution using GMRES by defining the action of $\mathbf{A}$ on a generic vector of moments $\vec{\theta}$ as

$$\mathbf{A}\vec{\theta} = \left(\mathbf{I} - \mathbf{DL}^{-1}\mathbf{MS}\right)\vec{\theta}. \tag{6.60}$$

To compute the action of $\mathbf{A}$, we first apply the S operator to the vector, convert the moments to angular fluxes using $\mathbf{M}$, perform a transport sweep on the resulting scattering source via the $\mathbf{L}^{-1}$ operator, and then convert the angular fluxes to moments via $\mathbf{D}$. The result is subtracted from the original vector. The way that the operators are defined, we can compute a scattering source, sweep

independently in each direction and compute a contribution to moments (as we did in source iteration), and do this for each direction. Note we only perform a transport sweep on the prescribed source once to get its contribution to the righthand side.

The convergence properties of GMRES are such that it converges faster for problems with less scattering, similar to source iteration, though in practice it always converges faster that source iteration on problems with any scattering. Another point is that although GMRES is guaranteed to converge, it will not necessary converge if we perform restarts. In restarted GMRES we delete the constructed Krylov subspace after m iterations, and use the approximate solution after m iterations as the initial guess for a new set of GMRES iterations. The upside of restarting is that we bound the storage of the algorithm at m vectors, however, convergence can be slowed or even not guaranteed for restarted GMRES with m too low.

6.7 CMFD for Discrete Ordinates

An alternative approach to source iteration is to use CMFD to accelerate the scattering source in source iteration. We will present the equations for 1-D CMFD acceleration of source iteration using the diamond difference spatial scheme, though the extension to 3-D is straightforward, except in notation.

We begin with an approximate value for the scattering source in the problem

and compute an updated angular flux using source iteration as

(6.61)

Using the $\ell + 1/2$ level angular fluxes we can compute the net current at each interface as

$$J_{i+1/2}^{\ell+1/2} = \sum_{n=1}^{N} w_n \mu_n \psi_n^{\ell+1/2}. \tag{6.62}$$

We then solve a system of diffusion equations of the form

$$\frac{\tilde{J}_{i+1/2}^{\ell+1} - \tilde{J}_{i-1/2}^{\ell+1}}{h_x} + \Sigma_{\mathrm{a}} \phi_i^{\ell+1} = \sum_{n=0}^{N} w_n q_{ni}, \tag{6.63}$$

where the currents are defined using Fick's law plus a correction as

$$\tilde{J}_{i+1/2}^{\ell+1} = -\hat{D}_{i+1/2} \frac{\phi_{i+1}^{\ell+1} - \phi_i^{\ell+1}}{h_x} - \tilde{D}_{i+1/2} \frac{\phi_{i+1}^{\ell+1} + \phi_i^{\ell+1}}{h_x}, \tag{6.64}$$

where $\hat{D}_{i+1/2}$ is the harmonic mean of the diffusion coefficients and $\tilde{D}_{i+1/2}$ is given by

$$\tilde{D}_{i+1/2} = \frac{J_{i+1/2}^{\ell+1/2} + \hat{D}_{i+1/2}(\phi_{i+1}^{\ell+1} - \phi_i^{\ell+1})}{\phi_{i+1}^{\ell+1} + \phi_i^{\ell+1}}. \tag{6.65}$$

We then go back to the source iteration step and use the scalar flux computed from Eq. (6.63) to given the scattering source for the next source iteration. We continue these iterations until the scalar flux solution converges. As in the nodal method, we expect this to converge more quickly because the CMFD solution gets a global coupling between all the scalar fluxes with the leakage from each zone corrected by transport, whereas the source iteration step gives an estimate of the first-collision source from a set of sources.