1 R-Z Geometry

Solving the transport equation in different coordinate systems may provide simpler ways of modeling a particular geometry or symmetry. In this section, we derive the R-Z transport equation to be solved. It assumes there is no variation in the azimuthal direction (of a cylinder), hence problems in R-Z geometry look very similar to problems in X-Y geometry. The streaming operator in cylindrical geometry is [?]

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi = \frac{\mu}{r} \frac{\partial}{\partial r}(r\psi) + \frac{\eta}{r} \frac{\partial \psi}{\partial \zeta} + \xi \frac{\partial \psi}{\partial z} - \frac{1}{r} \frac{\partial}{\partial \omega}(\eta \psi), \tag{1}$$

where $\boldsymbol{\Omega}$ is the direction of travel unit vector, ψ is the angular flux, and

$$\mu \equiv \boldsymbol{\Omega} \cdot \hat{e}_r = \sqrt{1-\xi^2} \cos \omega = \sin(\theta) \cos(\omega), \tag{2}$$

$$\eta \equiv \boldsymbol{\Omega} \cdot \hat{e}_\theta = \sqrt{1-\xi^2} \sin \omega = \sin(\theta) \sin(\omega), \tag{3}$$

$$\xi \equiv \boldsymbol{\Omega} \cdot \hat{e}_z = \cos(\theta). \tag{4}$$

The variables μ, η, ξ, ω, and θ are shown in the cylindrical coordinate system in Figure 1. We assume there is no solution variation in the azimuthal direction, i.e.

$$\frac{\partial \psi}{\partial \zeta} \equiv 0, \tag{5}$$

which simplifies the streaming term to

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi = \frac{\mu}{r} \frac{\partial}{\partial r}(r\psi) + \xi \frac{\partial \psi}{\partial z} - \frac{1}{r} \frac{\partial}{\partial \omega}(\eta \psi). \tag{6}$$

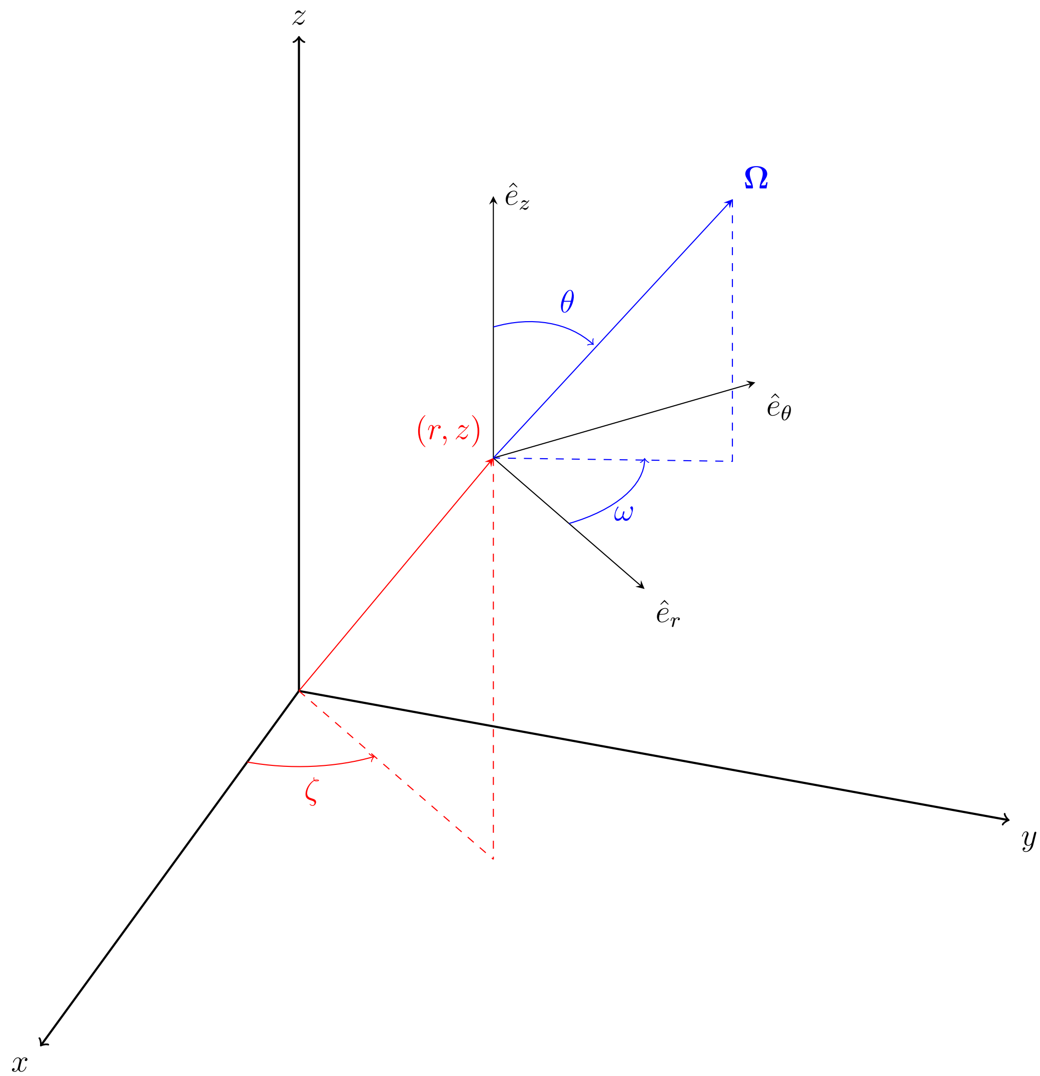

Figure 1: Cylindrical space-angle coordinate system showing the position (r, z) and direction of travel $\mathbf{\Omega}$.

The transport equation in R-Z geometry is then

$$\begin{aligned} &\frac{\mu}{r}\frac{\partial}{\partial r} r\psi\left(r, z, \mathbf{\Omega}\right) + \xi \frac{\partial}{\partial z}\psi\left(r, z, \mathbf{\Omega}\right) - \frac{1}{r}\frac{\partial}{\partial \omega}\eta\psi\left(r, z, \mathbf{\Omega}\right) + \sigma_t\left(r, z\right)\psi\left(r, z, \mathbf{\Omega}\right) \\ &\qquad = \frac{1}{4\pi}\int_{4\pi}\sigma_s\left(r, z\right) I\left(r, z, \mathbf{\Omega}'\right) d\Omega' + S_0\left(r, z, \mathbf{\Omega}\right) \end{aligned} \tag{7}$$

where σ_t is the total cross section, σ_s is the scattering cross section, and S_0 is an isotropic source as before.

1.1 Angular Discretization

Discretizing Equation 7 with a level-symmetric angular quadrature results in

$$\frac{\mu_{n,m}}{r}\frac{\partial}{\partial r}r\psi_{n,m}\left(r,z\right)+\xi_n\frac{\partial}{\partial z}\psi_{n,m}\left(r,z\right)-\frac{1}{r}\frac{\partial}{\partial \omega}\eta_{n,m}\psi_{n,m}\left(r,z\right)+\sigma_t\left(r,z\right)\psi_{n,m}\left(r,z\right)$$
$$=\frac{1}{4\pi}\int_{4\pi}\sigma_s\left(r,z\right)I\left(r,z,\mathbf{\Omega}'\right)d\Omega'+S_0\left(r,z,\mathbf{\Omega}\right) \quad (8)$$

for direction $\mathbf{\Omega}_{n,m}$, where index n describes a level of quadrature with constant ξ and the m index denotes the quadrature point on that level. The (n,m) indexing is shown in Figure 2.

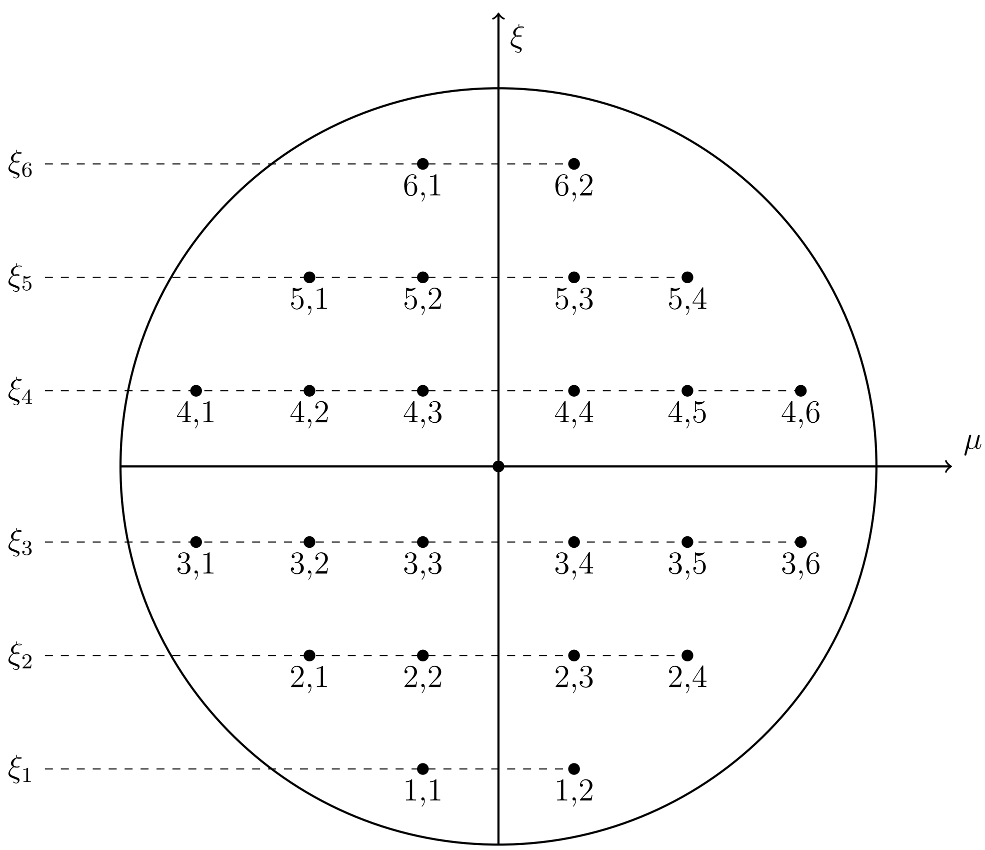

Figure 2: Angular discretization showing (ξ, μ) pairs; adapted from [**?**]

One of the major challenges is handling the anglar derivative term. Lewis and

Miller [?] describes an approximation for the partial derivative of the intensity with respect to ω:

$$-\frac{1}{r}\frac{\partial}{\partial\omega}\eta_{m,n}\psi_{n,m}\left(r,z\right)=\frac{\alpha^n_{m+1/2}\psi_{n,m+1/2}(r,z)-\alpha^n_{m-1/2}\psi_{n,m-1/2}(r,z)}{rw_{n,m}} \tag{9}$$

where $\alpha^n_{m+1/2}$ and $\alpha^n_{m-1/2}$ are angular differencing coefficients, and $w_{n,m}$ is the angular quadrature weight. We substitute this into Equation 18,

$$\begin{aligned}\frac{\mu_{n,m}}{r}\frac{\partial}{\partial r}r\psi_{n,m}\left(r,z\right)+\xi_n\frac{\partial}{\partial z}\psi_{n,m}\left(r,z\right)&\\+\frac{\alpha^n_{m+1/2}\psi_{m+1/2,n}(r,z)-\alpha^n_{m-1/2}\psi_{m-1/2,n}(r,z)}{rw_{n,m}}+\sigma_t\left(r,z\right)\psi_{n,m}\left(r,z\right)&\\=\frac{1}{4\pi}\int_{4\pi}\sigma_s\left(r,z\right)\psi\left(r,z,\mathbf{\Omega}'\right)d\Omega'+\frac{1}{4\pi}S_0\left(r,z\right)&\end{aligned} \tag{10}$$

Here, we pause to notice that there are similarities and differences between our Cartesian discretization. The absorption term, axial derivative term, and right-hand-side are the same in both coordinate systems. The differences arise in the radial and angular derivative terms.

After multiplying through by the radius r, the radial derivative term has a factor of r inside the derivative. The angular derivative term is also new and does not resemble a mass matrix so MFEM will require additional modification.

Requiring Equation 10 to satisfy the uniform infinite medium solution results in the condition,

$$\alpha^n_{m+1/2}=\alpha^n_{m-1/2}-\mu_{n,m}w_{n,m} \tag{11}$$

If $\alpha^n_{1/2}$ is known, then the remaining coefficients are uniquely determined. To find $\alpha^n_{1/2}$, we require that Equation 10 satisfy the conservation equation (Eq. 7). Given a quadrature set with an even number of $\mu_{n,m}$ values, setting $\alpha^n_{1/2}=0$ results in

$\alpha^n_{M_n+1/2} = 0$ per Equation 11 and the conservation equation is satisfied.

A relationship between $\psi_{n,m}$, $\psi_{n,m+1/2}$, and $\psi_{n,m-1/2}$ must be established. A weighted diamond difference scheme has been established by Morel and Montry [?],

$$\psi_{n,m}(r,z) = \tau_{n,m}\psi_{n,m+1/2} + \left(1-\tau_{n,m}\right)\psi_{n,m-1/2} \tag{12}$$

where $\tau_{n,m}$ linearly interpolates μ:

$$\tau_{n,m} = \frac{\mu_{n,m} - \mu_{n,m-1/2}}{\mu_{n,m+1/2} - \mu_{n,m-1/2}} \tag{13}$$

with

$$\mu_{n,m+1/2} = \sqrt{1-\xi_n^2}\cos\left(\varphi_{n,m+1/2}\right) \tag{14}$$

$$\varphi_{n,m+1/2} = \varphi_{n,m-1/2} + \pi\frac{w_{n,m}}{w_n} \tag{15}$$

$$w_n = \sum_{m=1}^{M_n} w_{n,m} \tag{16}$$

We take Equation 10, multiply through by r and perform a product rule on the radial derivative term,

$$\begin{aligned}\mu_{n,m}\left[\psi_{n,m}\left(r,z\right) + r\frac{\partial}{\partial r}\psi_{n,m}\left(r,z\right)\right] + r\xi_n\frac{\partial}{\partial z}\psi_{n,m}\left(r,z\right)\\ + \frac{\alpha^n_{m+1/2}\psi_{m+1/2,n}(r,z) - \alpha^n_{m-1/2}\psi_{m-1/2,n}(r,z)}{w_{n,m}} + r\sigma_t\left(r,z\right)\psi_{n,m}\left(r,z\right)\\ = \frac{r}{4\pi}\int_{4\pi}\sigma_s\left(r,z\right)\psi\left(r,z,\mathbf{\Omega}'\right)d\Omega' + \frac{r}{4\pi}S_0\left(r,z\right).\end{aligned} \tag{17}$$

We solve Equation 12 for $\psi_{n,m+1/2}$, perform a substitution, and move the known quantities to the right-hand-side,

$$\begin{aligned}\mu_{n,m} r \frac{\partial}{\partial r}\psi_{n,m}\left(r,z\right) + r\xi_n \frac{\partial}{\partial z}\psi_{n,m}\left(r,z\right) + \mu_{n,m}\psi_{n,m}\left(r,z\right) \\ + \frac{\alpha^n_{m+1/2}}{\tau_{n,m} w_{n,m}}\psi_{n,m}(r,z) + r\sigma_t\left(r,z\right)\psi_{n,m}\left(r,z\right) \\ = \frac{r}{4\pi}\int_{4\pi}\sigma_s\left(r,z\right)\psi\left(r,z,\mathbf{\Omega}'\right)d\Omega' + \frac{r}{4\pi}S_0\left(r,z\right) \\ + \left(\frac{1-\tau_{n,m}}{\tau_{n,m}}\frac{\alpha^n_{m+1/2}}{w_{n,m}} + \frac{\alpha^n_{m-1/2}}{w_{n,m}}\right)\psi_{n,m-1/2}(r,z). \quad (18)\end{aligned}$$

Given a level-symmetric quadrature set, all of the $\alpha^n_{n,m\pm 1/2}$ and $\tau_{n,m}$ values can be computed. We solve the starting direction equation to obtain $\psi_{n,1/2}$. That is, we solve the X-Y system for directions $\mathbf{\Omega}_{n,1/2}$,

$$\mathbf{\Omega}_{n,1/2}\cdot\mathbf{\nabla}\psi_{n,1/2} + \sigma_t\psi_{n,1/2} = \frac{1}{4\pi}\sigma_s\phi + \frac{1}{4\pi}S_0 \quad (19)$$

There is an alternate angular discretization method developed by Warsa and Prinja [**?**]. Instead of finding an approximation for the angular derivative, they perform a product rule:

$$\frac{\partial\psi}{\partial\omega} \equiv \frac{\partial\mu}{\partial\omega}\frac{\partial\psi}{\partial\mu} \quad (20)$$

Since,

$$\frac{\partial\mu}{\partial\omega} \equiv -\xi, \quad (21)$$

The angular derivative can be written

$$\frac{\partial\psi}{\partial\omega} \equiv -\xi\frac{\partial\psi}{\partial\mu} \quad (22)$$

Here, an approximation for the μ-derivative must be established.

1.2 Spatial Discretization

The finite element discretization is performed here. The methodology is similar to the Cartesian geometry. First, we subdivide a problem domain using a spatial mesh. Then, we multiply Equation 18 by a test function and integrate over the volume of a single mesh zone,

$$\begin{aligned}(r\boldsymbol{\Omega}_{n,m}\cdot\boldsymbol{\nabla}\psi_{n,m},v_i)_{\mathbb{D}}&+(\mu_{n,m}\psi_{n,m},v_i)_{\mathbb{D}}\\&+\left(\frac{\alpha^n_{m+1/2}}{\tau_{n,m}w_{n,m}}\psi_{n,m},v_i\right)_{\mathbb{D}}+(r\sigma_t\psi_{n,m},v_i)_{\mathbb{D}}\\&=\left(\frac{r}{4\pi}\int_{4\pi}\sigma_s\psi d\Omega',v_i\right)_{\mathbb{D}}+\left(\frac{r}{4\pi}S_0,v_i\right)_{\mathbb{D}}\\&\quad+\left(\left(\frac{1-\tau_{n,m}}{\tau_{n,m}}\frac{\alpha^n_{m+1/2}}{w_{n,m}}+\frac{\alpha^n_{m-1/2}}{w_{n,m}}\right)\psi_{n,m-1/2},v_i\right)_{\mathbb{D}},\end{aligned}\tag{23}$$

where the Cartesian gradient operator is used and the inner product notation,

$$(a,b)_{\mathbb{D}}\equiv\int_{\mathbb{D}}ab,\tag{24}$$

is used. We perform an integration by parts,

$$\begin{aligned}(r\boldsymbol{\Omega}_{n,m}\cdot\hat{n}\psi_{n,m},v_i)_{\partial\mathbb{D}}&-(r\psi_{n,m},\boldsymbol{\Omega}_{n,m}\cdot\boldsymbol{\nabla}v_i)_{\mathbb{D}}+(\mu_{n,m}\psi_{n,m},v_i)_{\mathbb{D}}\\&+\left(\frac{\alpha^n_{m+1/2}}{\tau_{n,m}w_{n,m}}\psi_{n,m},v_i\right)_{\mathbb{D}}+(r\sigma_t\psi_{n,m},v_i)_{\mathbb{D}}\\&=\left(\frac{r}{4\pi}\int_{4\pi}\sigma_s\psi d\Omega',v_i\right)_{\mathbb{D}}+\left(\frac{r}{4\pi}S_0,v_i\right)_{\mathbb{D}}\\&\quad+\left(\left(\frac{1-\tau_{n,m}}{\tau_{n,m}}\frac{\alpha^n_{m+1/2}}{w_{n,m}}+\frac{\alpha^n_{m-1/2}}{w_{n,m}}\right)\psi_{n,m-1/2},v_i\right)_{\mathbb{D}},\end{aligned}\tag{25}$$

to obtain our angular and spatially discretized R-Z transport equation.

1.3 Lumping

1.4 DSA

1.5 Symmetry Preservation

1.6 Other

1.7 Reflecting Boundary Conditions

To incorporate reflecting boundary conditions, we will "guess" the incident angular fluxes, update them with outgoing angular fluxes from the previous iteration, and adapt a convergence criterion for those fluxes. Along the z-axis, the reflection for direction $\mathbf{\Omega} = (\mu, \eta, \xi)$ is $\mathbf{\Omega}_R = (-\mu, \eta, \xi)$.