Neutron transport theory and discrete ordinates method For structural grid systems in Cartesian coordinate system

Xingguang Zhou¹

¹Nuclear Thermal-hydraulics Laboratory Xi'an Jiaotong University

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- $lue{1}$ Neutron transport equation and S_N
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Physical quantities and their relationships

Neutron angular flux (unit: ${\rm cm}^{-2}\cdot {\rm s}^{-1}$)

$$\phi\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) = V \cdot N\left(\mathbf{r}, \mathbf{\Omega}, E, t\right).$$

Neutron scalar flux (unit: $cm^{-2} \cdot s^{-1}$)

$$\Phi(\mathbf{r}, E, t) = \int_0^{4\pi} \phi(\mathbf{r}, \mathbf{\Omega}, E, t) d\mathbf{\Omega}.$$

Neutron angular current density (unit: $cm^{-2} \cdot s^{-1}$)

$$\mathbf{J}\left(\mathbf{r},\mathbf{\Omega},E,t\right) = \mathbf{\Omega} \cdot \phi\left(\mathbf{r},\mathbf{\Omega},E,t\right).$$

Neutron current density (unit: $cm^{-2} \cdot s^{-1}$)

$$\mathbf{J}(\mathbf{r}, E, t) = \int_{0}^{4\pi} \mathbf{J}(\mathbf{r}, \mathbf{\Omega}, E, t) \, \mathrm{d}\mathbf{\Omega}.$$

Generalized derivation of neutron transport equation

According to the neutron balance and Reynolds transport theorem, we can get the generalized form of neutron transport equation,

$$\frac{D}{Dt} \int_{\mathbb{V}} N(\mathbf{r}, \mathbf{\Omega}, E, t) d^{3}r = \frac{\partial}{\partial t} \int_{\mathbb{V}} N(\mathbf{r}, \mathbf{\Omega}, E, t) d^{3}r
+ \oint_{\mathbb{S}} \mathbf{n} \cdot \mathbf{V} \otimes N(\mathbf{r}, \mathbf{\Omega}, E, t) d^{2}r,$$

where ${\bf n}$ is the unit normal vector of the surface, and ${\bf V}={\bf \Omega} V.$ Hence the equation can be rewritten as

$$\frac{D}{Dt} \int_{\mathbb{V}} N(\mathbf{r}, \mathbf{\Omega}, E, t) d^{3}r = \frac{\partial}{\partial t} \int_{\mathbb{V}} N(\mathbf{r}, \mathbf{\Omega}, E, t) d^{3}r + \oint_{\mathbb{S}} \mathbf{n} \cdot \mathbf{\Omega} \otimes \phi(\mathbf{r}, \mathbf{\Omega}, E, t) d^{2}r.$$

Generalized derivation of neutron transport equation

Considering the source terms and using Gauss theorem, we can get

$$\frac{\partial}{\partial t} \int_{\mathbb{V}} N\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) \mathrm{d}^3 r + \int_{\mathbb{V}} \nabla \cdot \mathbf{\Omega} \phi\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) \mathrm{d}^3 r = \int_{\mathbb{V}} Q\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) \mathrm{d}^3 r.$$

The conservative neutron transport equation can be obtained by removing the volume integration,

$$\frac{\partial}{\partial t} N(\mathbf{r}, \mathbf{\Omega}, E, t) + \nabla \cdot \mathbf{\Omega} \phi(\mathbf{r}, \mathbf{\Omega}, E, t) = Q(\mathbf{r}, \mathbf{\Omega}, E, t).$$

The above equation still be rewritten into a form with more explicit physical meaning,

$$\frac{\partial}{\partial t} N\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) + \nabla \cdot \mathbf{J}\left(\mathbf{r}, \mathbf{\Omega}, E, t\right) = Q\left(\mathbf{r}, \mathbf{\Omega}, E, t\right).$$

Generalized derivation of neutron transport equation

Hence, the conversative form of neutron transport equation with isotropic fission source in critical problem is

$$\nabla \cdot \mathbf{J} (\mathbf{r}, \mathbf{\Omega}, E) = -\Sigma_{t} (\mathbf{r}, E) \phi (\mathbf{r}, \mathbf{\Omega}, E)$$

$$+ \int_{0}^{4\pi} d\mathbf{\Omega}' \int_{0}^{\infty} dE' \Sigma_{s} (\mathbf{r}, \mathbf{\Omega} \to \mathbf{\Omega}', E' \to E') \phi (\mathbf{r}, \mathbf{\Omega}', E')$$

$$+ \frac{\chi(E)}{4\pi k_{eff}} \int_{0}^{\infty} dE' \nu \Sigma_{f} (\mathbf{r}, E') \int_{0}^{4\pi} \phi (\mathbf{r}, \mathbf{\Omega}', E') d\mathbf{\Omega}',$$

where

$$\mathbf{J}\left(\mathbf{r},\mathbf{\Omega},E\right) = \mathbf{\Omega}\phi\left(\mathbf{r},\mathbf{\Omega},E\right)$$

Discrete ordinates method - S_N

In neutron transport equation, there are four types arguments which are need to be solved, angular argument Ω , spatial argument \mathbf{r} , neutron energy E, and time t.

The most important argument for neutron transport equation is angular argument Ω , and actually Ω comes from the Boltzmann equation, which also can be used in radiative heat transfer. Discrete ordinates Method (S_N) is a popular method for solve Ω , that is first proposed by Chandrasekhar to calculate the radiation and heat transfer of celestical bodies in the universe.

Since S_N has the clear physical meaning, we use S_N to discretize Ω in neutron transport equation.

Discrete ordinates method - S_N

With the help of Gaussian integration , the integration of neutron angular flux to Ω can be derived as

$$\psi\left(\mathbf{r},E,t\right) = \int_{0}^{4\pi} \phi\left(\mathbf{r},\mathbf{\Omega},E,t\right) d\mathbf{\Omega} = \sum_{m=1}^{M} \omega_{m} \phi\left(\mathbf{r},\mathbf{\Omega}_{m},E,t\right),$$

where ω_m is the weight in Gaussian integration. Hence, if we want to discretize the Ω in Cartesian coordinate system from $\Omega_{m-\frac{1}{2}}$ to $\Omega_{m+\frac{1}{2}}$, we can get

$$\int_{\mathbf{\Omega}_{m-\frac{1}{2}}}^{\mathbf{\Omega}_{m+\frac{1}{2}}} \phi(\mathbf{r}, \mathbf{\Omega}, E, t) d\mathbf{\Omega} = \omega_m \phi(\mathbf{r}, \mathbf{\Omega}_m, E, t).$$

In Cartesian coordinate system, the convective term can be written as

Discrete ordinates method - S_N

For $\Omega\cdot
abla \phi$, we also can derive the discretization of Ω from $\Omega_{m-\frac{1}{2}}$ to $\Omega_{m+\frac{1}{2}}$ in Cartesian coordinate system, as

$$\int_{\mathbf{\Omega}_{m-\frac{1}{2}}}^{\mathbf{\Omega}_{m+\frac{1}{2}}} \mathbf{\Omega} \cdot \nabla \phi \left(\mathbf{r}, \mathbf{\Omega}, E, t \right) d\mathbf{\Omega} = \omega_m \mathbf{\Omega}_m \cdot \nabla \phi \left(\mathbf{r}, \mathbf{\Omega}_m, E, t \right).$$

Why we always alert "Cartesian coordinate system"? This is because only in Cartesian coordinate system, which does not contain the leakage term (part of neutron flux) due to coordinate change, above operation of discretization of Ω is established in such a way like "integral mean value theorem".

$$\int_{\mathbf{\Omega}_{m-\frac{1}{2}}}^{\mathbf{\Omega}_{m+\frac{1}{2}}} \mathbf{\Omega} \cdot \nabla \phi \left(\mathbf{\Omega}\right) d\mathbf{\Omega} = \omega_m \mathbf{\Omega}_m \cdot \nabla \phi \left(\mathbf{\Omega}_m\right)$$
$$= \mathbf{\Omega}_{m'} \cdot \nabla \phi \left(\mathbf{\Omega}_{m'}\right) \left|\mathbf{\Omega}_{m+\frac{1}{2}} - \mathbf{\Omega}_{m-\frac{1}{2}}\right|.$$

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Actually, in neutron transport equation, one-dimensional condition and two-dimensional condition are both the special cases of three-dimensional condition. The integrals of the independent angle variables are

1). one-dimensional ("only polar angle $\theta \in [0, \pi]$ ")

$$\frac{1}{2\pi} \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta = 2 \Rightarrow \int_0^{\pi} \sin\theta d\theta,$$

2). two-dimensional (azimuthal angle $\varphi \in [0,2\pi]$, polor angle $\theta \in [0,\pi/2]$)

$$\frac{1}{2} \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta = 2\pi \Rightarrow \int_0^{2\pi} d\varphi \int_0^{\frac{\pi}{2}} \sin\theta d\theta,$$

3). three-dimensional (azimuthal angle $\varphi \in [0,2\pi]$, polor angle $\theta \in [0,\pi]$)

$$\int_0^{2\pi} \mathrm{d}\varphi \int_0^{\pi} \sin\theta \, \mathrm{d}\theta = 4\pi.$$

However, the integrals of the independent angle variables are not the total integrals. In fact, we still get

$$\sum_{m=1}^{M_{(1)}} \omega_{m_{(1)}} = \frac{1}{2\pi} \sum_{m=1}^{M_{(3)}} \omega_m = 2, \quad \sum_{m=1}^{M_{(2)}} \omega_{m_{(2)}} = \frac{1}{2} \sum_{m=1}^{M_{(3)}} \omega_m = 2\pi,$$

for 1-D, 2-D, and 3-D, respectively. In most context of neutron transport equation, the increment solid angle $\mathrm{d}\Omega$ is usually defined as

$$\mathrm{d}\mathbf{\Omega} = \frac{\mathrm{d}\varphi}{2\pi} \frac{\sin\theta \mathrm{d}\theta}{2},$$

to yield the convenient normalization over all angles

$$\int_0^{4\pi} \mathrm{d} \mathbf{\Omega} = \int_0^{2\pi} \frac{\mathrm{d} \varphi}{2\pi} \int_0^{\pi} \frac{\sin \theta \mathrm{d} \theta}{2} = 1.$$

After the normalization of $d\Omega$, for 1-D, 2-D, and 3-D, that

$$\int_0^{4\pi} \mathrm{d}\mathbf{\Omega} = \sum_{m=1}^M \omega_m = 1.$$

The reason we consider that normalization of $d\Omega$ is that we need to use Gaussian quadrature set in S_N method.

From the **Numerical Analysis**, we can know that usually $\sum \omega_m = 1$ or 2 in Gaussian quadrature set. It is rarely and hard to make $\sum \omega_m = 4\pi$, which means that Gaussian integral points also need to be re-designed. In the other words, the quadrature sets with $\sum \omega_m = 1$ or 2 are very mature. Hence, we make the normalization of $\mathrm{d}\Omega$ to adapt Gaussian quadrature set.

In addition, there are some other physical considerations, which will make the computational load much lesser, accroding to "old" computers.

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For isotropic fission source in steady-state critical problems, we always get

$$Q_{f}\left(\mathbf{r},\mathbf{\Omega},E\right) = \frac{\chi\left(E\right)}{4\pi k_{eff}} \int_{0}^{\infty} dE' \int_{0}^{4\pi} d\mathbf{\Omega}' \nu \Sigma_{f}\left(E'\right) \phi\left(\mathbf{r},\mathbf{\Omega}',E'\right),$$

if we use the normalization of $d\Omega$, Q_f can be written as

$$Q_f(\mathbf{r}, \mathbf{\Omega}, E) = \frac{\chi(E)}{k_{eff}} \int_0^\infty dE' \int_0^{4\pi} \frac{d\mathbf{\Omega'}}{4\pi} \nu \Sigma_f(E') \phi(\mathbf{r}, \mathbf{\Omega'}, E')$$
$$= \frac{\chi(E)}{k_{eff}} \int_0^\infty dE' \nu \Sigma_f(E') \sum_{m=1}^M \frac{\omega_m}{4\pi} \phi(\mathbf{r}, \mathbf{\Omega'}_m, E').$$

We can see that 4π is integrated in the quadrature weight ω_m , and then the identity of the Q_f is unchanged. This identity transformation also meets the requirements of existing Gaussian quadrature sets.

For scattering source term in steady-state critical problems, we usually use "isotropic" scattering, as

$$Q_s(\mathbf{r}, \mathbf{\Omega}, E) = \frac{1}{2\pi} \int_0^\infty dE' \int_0^{4\pi} d\mathbf{\Omega}' \Sigma_s \left(\mathbf{r}, \underbrace{\mathbf{\Omega}' \cdot \mathbf{\Omega}}_{\mu_0}, E' \to E \right) \phi\left(\mathbf{r}, \mathbf{\Omega}', E' \right).$$

We can expanse the scattering macro-scopic with Legendre expansions, as

$$\Sigma_{s}\left(\mathbf{r},\mu_{0},E'\to E\right) = \sum_{l=0}^{\infty} \frac{2l+1}{2} \Sigma_{s,l}\left(\mathbf{r},E'\to E\right) P_{l}\left(\mu_{0}\right),$$

if l=0, then we get the "isotropic" scattering source term,

$$Q_s(\mathbf{r}, \mathbf{\Omega}, E) = \int_0^\infty \frac{1}{4\pi} \Sigma_s(\mathbf{r}, E' \to E) \int_0^{4\pi} \phi(\mathbf{r}, \mathbf{\Omega}', E') d\mathbf{\Omega}' dE',$$

$$Q_{s}(\mathbf{r}, \mathbf{\Omega}, E) = \int_{0}^{\infty} \frac{1}{4\pi} \Sigma_{s} \left(\mathbf{r}, E' \to E \right) \sum_{m=1}^{M} \omega_{m} \phi \left(\mathbf{r}, \mathbf{\Omega}_{m}, E' \right) dE'$$
$$= \int_{0}^{\infty} \Sigma_{s} \left(\mathbf{r}, E' \to E \right) \sum_{m=1}^{M} \frac{\omega_{m}}{4\pi} \phi \left(\mathbf{r}, \mathbf{\Omega}_{m}, E' \right) dE'.$$

From the above discussions, we can clearly know that if we use S_N method with Gaussian integraions, multiplication factors (such as $4\pi)$ can be introduced to maintain the $\sum \omega_m = 1.$ And the Gaussian integral points Ω_m do not need to be changed. Hence the source terms as Q_s and Q_f are need to be re-written into the identity form. After the above identity transformation, the "real" neutron (angular) scalar flux can be calculated.

For the isotropic source terms in 1-D problem with single group, we can get

$$\mu \frac{\partial \phi(z, \mathbf{\Omega})}{\partial z} + \Sigma_t(z) \phi(z, \mathbf{\Omega}) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi' \int_1^{-1} \Sigma_s(z, \mu_0) \phi(z, \mathbf{\Omega}') d\mu' + \frac{1}{4\pi k_{eff}} \nu \Sigma_f \Phi(z),$$

where $\mu_0 = \Omega' \cdot \Omega$. With the basic principle of symmetry, the equation can be re-written into

$$\mu \frac{\partial \phi(z, \mu)}{\partial z} + \Sigma_t(z) \phi(z, \mu) = \int_1^{-1} \Sigma_s(z, \mu_0) \phi(z, \mu') d\mu' + \frac{1}{2 \cdot k_{eff}} \nu \Sigma_f \Phi(z),$$

where $\phi\left(z,\mathbf{\Omega}'\right)=\frac{1}{2\pi}\phi\left(z,\mu'\right)$, and $\Sigma_{s}\left(z,\mathbf{\Omega}'\to\mathbf{\Omega}\right)=\frac{1}{2\pi}\Sigma_{s}\left(z,\mu_{0}\right)$

With the isotropic source terms, the final 1-D problem with single group can be written as

$$\mu \frac{\partial \phi \left(z,\mu \right) }{\partial z} + \Sigma_{t} \left(z \right) \phi \left(z,\mu \right) = \frac{1}{2} \Sigma_{s} \left(z \right) \Phi \left(z \right) + \frac{1}{2} \frac{1}{k_{eff}} \nu \Sigma_{f} \Phi \left(z \right). \label{eq:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equation:equat$$

Hence, $\Phi\left(z\right)=\sum_{m=1}^{M}\omega_{m}\phi\left(r,\mu_{m}\right)$. We suppose that move $\frac{1}{2}$ into ω_{m} to ensure that $\sum_{m=1}^{M}\omega_{m}=1$. Therefore, the equation in the code for 1-D critical problem can be written as

$$\mu \frac{\partial \phi\left(z,\mu\right)}{\partial z} + \Sigma_{t} \phi\left(z,\mu\right) = \Sigma_{s} \sum_{m=1}^{M} \omega_{m} \phi\left(z,\mu_{m}\right) + \frac{\nu \Sigma_{f}}{k_{eff}} \sum_{m=1}^{M} \omega_{m} \phi\left(z,\mu_{m}\right).$$

$$\sum_{m=1}^{M} \omega_m = 1$$

Descretization of the above equation with S_N method, we can get

$$\mu_{m} \frac{\partial \phi_{m}\left(z\right)}{\partial z} + \Sigma_{t} \phi_{m}\left(z\right) = \Sigma_{s} \sum_{m=1}^{M} \omega_{m} \phi\left(z, \mu_{m}'\right) + \frac{\nu \Sigma_{f}}{k_{eff}} \sum_{m=1}^{M} \omega_{m} \phi_{m}\left(z\right),$$

and also use FVM to descretize the spatial parameters, as

$$\mu_m \left(\phi_{i + \frac{1}{2}, m} - \phi_{i - \frac{1}{2}, m} \right) + \Sigma_{t, i} \phi_{i, m} \Delta z = \left(\Sigma_{s, i} + \frac{\nu \Sigma_{f, i}}{k_{eff}} \right) \sum_{m=1}^{M} \omega_m \phi_{i, m} \Delta z.$$

Let

$$Q_{i,m} = \left(\Sigma_{s,i} + \frac{\nu \Sigma_{f,i}}{k_{eff}}\right) \sum_{m=1}^{M} \omega_m \phi_{i,m}$$

Hence

$$\mu_m \left(\phi_{i+\frac{1}{2},m} - \phi_{i-\frac{1}{2},m} \right) + \Sigma_{t,i} \phi_{i,m} \Delta z = \mathcal{Q}_{i,m} \Delta z.$$

With the central difference, we can get

$$\begin{cases} \phi_{i+\frac{1}{2},m} = 2\phi_{i,m} - \phi_{i-\frac{1}{2},m}, & \mu_m > 0 \\ \phi_{i-\frac{1}{2},m} = 2\phi_{i,m} - \phi_{i+\frac{1}{2},m}, & \mu_m < 0, \end{cases}$$

and first-order upwind sheme

$$\begin{cases} \phi_{i+\frac{1}{2},m} = \phi_{i,m}, & \mu_m > 0 \\ \phi_{i-\frac{1}{2},m} = \phi_{i,m}, & \mu_m < 0, \end{cases}$$

substituting the scheme into the equation, we can get the solution of the iteration.

Solution of central difference and first-order upwind scheme

$$\begin{split} \phi_{i,m} &= \frac{\mathcal{Q}_{i,m}, \Delta z + C \mu_m \phi_{i-\frac{1}{2},m}}{C \mu_m + \Sigma_{t,i} \Delta z}, \quad \mu_m > 0, \\ \phi_{i,m} &= \frac{\mathcal{Q}_{i,m}, \Delta z - C \mu_m \phi_{i+\frac{1}{2},m}}{-C \mu_m + \Sigma_{t,i} \Delta z}, \quad \mu_m < 0, \end{split}$$

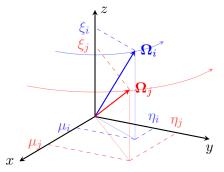
where, ${\cal C}=2$ in central difference scheme, and ${\cal C}=1$ in first-order upwind scheme.

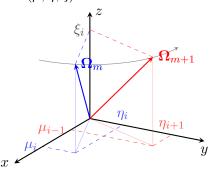
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Ω and its properties

 $\mu = \Omega \cdot \mathbf{e}_x$, $\eta = \Omega \cdot \mathbf{e}_y$, $\xi = \Omega \cdot \mathbf{e}_z$ are the projections of angular parameter Ω . It means that Ω can be written as $\Omega = (\mu, \eta, \xi)$.





$$\begin{split} \mu^2 + \eta^2 + \xi^2 &= 1, \quad \mu_i^2 + \eta_i^2 + \xi_i^2 = 1, \\ \Rightarrow \quad \mu_{i-1}^2 + \eta_{i+1}^2 + \xi_i^2 &= 1. \end{split}$$

Ω and its properties

 ${\bf \Omega}$ and Gaussian quadrature set also have the following properties. For $\phi\left({\bf r},{\bf \Omega}\right)=1,$ that

$$\Phi(\mathbf{r}) = \int_0^{4\pi} \phi(\mathbf{r}, \mathbf{\Omega}) d\mathbf{\Omega} = \sum_{m=1}^M \omega_m \phi(\mathbf{r}, \mathbf{\Omega}_m) = 4\pi.$$

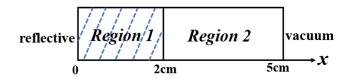
With the isotropic neutron angular flux, that

$$\mathbf{J}\left(\mathbf{r}\right) = \int_{0}^{4\pi} \mathbf{J}\left(\mathbf{r}, \mathbf{\Omega}\right) = \sum_{m=1}^{M} \omega_{m} \mathbf{\Omega}_{m} \phi_{C}\left(\mathbf{r}, \mathbf{\Omega}_{m}\right) = \mathbf{0} \Rightarrow \sum_{m=1}^{M} \omega_{m} \mathbf{\Omega}_{m} = \mathbf{0}.$$

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Problem description



Group constants of Region 1

$$\Sigma_t = 1.0 \text{ cm}^{-1}, \quad \Sigma_s = 0.5 \text{ cm}^{-1}, \quad \nu \Sigma_f = 1.0 \text{ cm}^{-1}.$$

Group constants of Region 2

$$\Sigma_t = 0.8 \text{ cm}^{-1}, \quad \Sigma_s = 0.4 \text{ cm}^{-1}, \quad \nu \Sigma_f = 0.0 \text{ cm}^{-1}.$$

Use S8 method to solve this problem with central difference scheme and first-order upwind sheme.

Data structure and algorithm

Algorithm 1 solve $\phi_{i,m}$, $\mu_m > 0$

```
Require: \phi_{i,m}, boundary, \phi_{i,m}^{User}
  1: while m \in [1, M], \mu_m > 0 do
            while i \in [1, I] do
                 if Reflective then
  3:
                      \phi_{i,m} \Rightarrow \phi_{i,M-m+1}
  4:
                 else
  5:
                      \phi_{i,m} \Rightarrow \phi_{i,m}^{User}
  6:
                \begin{array}{l} \text{end if} \\ \phi_{i,m} = \frac{\mathcal{Q}_{i,m}, \Delta z + C \mu_m \phi_{i-\frac{1}{2},m}}{C \mu_m + \Sigma_{t,i} \Delta z} \end{array}
  7:
  8:
                 \phi_{i,m+\frac{1}{2}} \Leftarrow C\phi_{i,m} - (C-1)\phi_{i,m-\frac{1}{2}}
  9.
                 call NegativeFluxCorrection
10:
            end while
```

Algorithm 2 solve $\phi_{i,m}$, $\mu_m < 0$

```
Require: \phi_{i,m}, boundary, \phi_{i,m}^{User}
  1: while m \in [1, M], \mu_m < 0 do
          while i \in [1, I] do
               if Reflective then
  3:
                    \phi_{i.m} \Rightarrow \phi_{i.M-m+1}
  4:
               else
  5:
                   \phi_{i,m} \Rightarrow \phi_{i,m}^{User}
  6:
  7:
               end if \phi_{i,m} = \frac{\mathcal{Q}_{i,m}, \Delta z - C\mu_m\phi_{i+\frac{1}{2},m}}{-C\mu_m + \Sigma_{t,i}\Delta z}
  8:
  9.
               \phi_{i,m-\frac{1}{2}} \Leftarrow C\phi_{i,m} - (C-1)\phi_{i,m+\frac{1}{2}}
               call NegativeFluxCorrection
10:
           end while
11:
12: end while
```

12: end while

11:

Data structure and algorithm

Algorithm 3 source term

Require: $\phi_{i,m}, k_{eff}$

1: while
$$m \in [1, M]$$
 do

2: while
$$i \in [1, I]$$
 do

3:
$$\Phi_i \Leftarrow 0$$

4: **while**
$$m' \in [1, M]$$
 do
5: $\Phi_i \Leftarrow \sum_{m'}^M \omega_{m'} \phi_{i,m'}$

5:
$$\Phi_i \Leftarrow \sum_{m'}^{M} \omega_{m'} \phi_{i,m'}$$

6: end while

7:
$$Q_{i,m} \Leftarrow \left(\Sigma_{s,i} + \frac{\nu \Sigma_{f,i}}{k_{eff}}\right) \Phi_i$$

end while 8.

end while

Algorithm 4 eigenvalue

Require:
$$\Phi_i$$
, Φ_i^{Old} , k_{eff}^{Old}

1:
$$Q_f \Leftarrow \sum_{i=1}^I \nu \Sigma_i \Phi_i$$

2:
$$\mathcal{Q}_f^{Old} \Leftarrow \sum_{i=1}^{I} \nu \Sigma_i \Phi_i^{Old}$$

3:
$$k_{eff} = \frac{\mathcal{Q}_f \cdot k_{eff}^{Old}}{\mathcal{Q}_f^{Old}}$$

Data structure and algorithm

Algorithm 5 power iteration

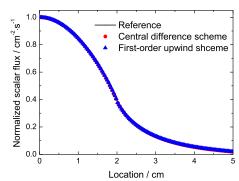
```
Require: \phi_{i,m}, boundary, k_{eff}
 1: call MeshGeneration
 2: call Initialization
 3: while iter \in [1, iMAX] do
       call SourceTerm
 4:
    call Solve \phi_{i,m}, \mu_m < 0
     call Solve \phi_{i,m}, \mu_m > 0
 6:
      call EigenValue
       if \left|k_{eff}-k_{eff}^{Old}\right|<1.e-6 then
 8:
           return
10:
      end if
     \phi_{i,m}^{Old} \Leftarrow \phi_{i,m}
11:
       k_{eff}^{Old} \Leftarrow k_{eff}
12:
```

13: end while

Result and discussion

Table 1: Comparison of k_{eff}

Method	k_{eff}	Deviation
MCNP	1.67869	-
S8-CD	1.68169	+300 pcm
S8-FUD	1.67837	-32 pcm



The results show that S8 method with central difference and first-order upwind schemes are both can calculation the ISSA problem correctly. We use 100 nodes in CD scheme and 150 nodes in FUD scheme, that in second order accuracy and first order accuracy, respectively.

Conclusion

- Based on the conservation of neutron number and the basic physical meaning of each physical quantity, we deduced the neutron transport equation.
- Symmetry and discrete ordinate method in neutron transport equation are introduced.
- Finally, we code the S8 to solve ISSA benchmark with Fortran 90. The results show that in the deterministic neutronics calculation, grid system, discretized angle and scheme accuracy are all related, and the characteristics such as error cancellation need to be considered.

Thanks for your attention!

zxg818@stu.xjtu.edu.cn