

Discrete Ordinates

Edward Norris

April 8, 2016

Abstract

The abstract text goes here.

Contents

1 CODE	2
2 Introduction	5
3 Mathematical Development	5
3.1 The Boltzmann Equation	5
3.2 Harmonic Approximation	5
3.3 Discretization	6
4 Implementation	7
4.1 Design	7
4.2 Language Selection	8
4.3 Salome	8
4.4 Framework Integration	8
4.5 C++ Implementation	8
5 MPI Implementation	8
6 GPU Implementation	8
7 Conclusion	9
8 Appendix	9
8.1 Laplace's Equation	9
8.2 Legendre Polynomials	10
8.3 Spherical Harmonic Function	10
8.4 Klein-Nishina Formula	13
8.5 Numeric Integration	13

1 CODE

Consider that we have the following variables, Ψ which is a function of x, y, z, E , and $\hat{\Omega}$. Further, we have the in-flux variables Ψ_{x-in}, Ψ_{y-in} , and Ψ_{z-in} .

Given:

- A list of all energies, \mathcal{E}
- A list of all directions in the quadrature, Q
- A mapping from r to zone number, $\mathcal{Z}(r)$
- Lists of direction cosines, μ, ξ , and η
- A map of r to voxel volume, $V(r)$
- A list of all x, y , and z voxel centers, X, Y , and Z
- A list of weights for the quadrature, ω
- A list of scatter cross sections in zone $\mathcal{Z}(r)$ from energy E' to E , $\Sigma_s(\mathcal{Z}(r), E', E)$
- A list of total cross sections in zone $\mathcal{Z}(r)$ at energy E , $\Sigma_T(\mathcal{Z}(r), E)$
- The surface area of all voxels, $A_{xy}(r), A_{yz}(r), A_{xz}(r)$

```

1 function sweep()
3    $\phi(r, E) = \vec{0}$     # Scalar flux
4    $\Psi(r, \Omega, E) = \vec{0}$   # Angular flux
5
6   for  $E \in \mathcal{E}$  in descending order
7     while not converged
8       for  $\Omega \in Q$  in any order
9         if  $\mu(\Omega) > 0$  and  $\xi(\Omega) > 0$  and  $\eta(\Omega) > 0$ 
10          octant1()
11        else if  $\mu(\Omega) > 0$  and  $\xi(\Omega) > 0$  and  $\eta(\Omega) < 0$ 
12          octant2()
13        ...
14      else
15        octant8()

```

```

1  function octant1()
3    for  $x \in X$  in ascending order
5      for  $y \in Y$  in ascending order
7        for  $z \in Z$  in ascending order
9           $S = \text{totalScatter}(x, y, z, \Omega, E)$ 
11         # Get the in-flux from the previous out-flux
13          $\Psi_{x-in}(x, y, z, E, \Omega) \leftarrow \Psi_{x-out}(x - \Delta x, y, z, E, \Omega)$ 
15          $\Psi_{y-in}(x, y, z, E, \Omega) \leftarrow \Psi_{x-out}(x, y - \Delta y, z, E, \Omega)$ 
17          $\Psi_{z-in}(x, y, z, E, \Omega) \leftarrow \Psi_{x-out}(x, y, z - \Delta z, E, \Omega)$ 
19         # Calculate the angular flux
21          $n \leftarrow S + 2\mu(\Omega)A_{yz}(y, z)\Psi_{x-in}(x, y, z, E, \Omega) +$ 
23              $2\xi(\Omega)A_{xz}(x, z)\Psi_{y-in}(x, y, z, E, \Omega) +$ 
25              $2\eta(\Omega)A_{xy}(x, y)\Psi_{z-in}(x, y, z, E, \Omega)$ 
d  $\leftarrow 2\mu(\Omega)A_{yz}(y, z) + 2\xi(\Omega)A_{xz}(x, z) + 2\eta(\Omega)A_{xy}(x, y) + \Sigma_T(\mathcal{Z}(r), E)$ 
 $\Psi(x, y, z, E, \Omega) \leftarrow n/d$ 
27         # Calculate the out-flux
 $\Psi_{x-out}(x, y, z, E, \Omega) \leftarrow 2\Psi(x, y, z, E, \Omega) - \Psi_{x-in}(x, y, z, E, \Omega)$ 
 $\Psi_{y-out}(x, y, z, E, \Omega) \leftarrow 2\Psi(x, y, z, E, \Omega) - \Psi_{y-in}(x, y, z, E, \Omega)$ 
 $\Psi_{z-out}(x, y, z, E, \Omega) \leftarrow 2\Psi(x, y, z, E, \Omega) - \Psi_{z-in}(x, y, z, E, \Omega)$ 
# Increment the scalar flux
 $\phi(x, y, z, E) \leftarrow \phi(x, y, z, E) + \omega(\Omega)\Psi(x, y, z, E, \Omega)$ 

```

```

1 function totalScatter( $r, \Omega, E$ )
2
3     # Assume a point source at  $r_0$  with energy  $E_0$  and strength  $S_0$ 
4         particles / sec
5          $S_x \leftarrow 0$ 
6         if  $r = r_0$  and  $E = E_0$ 
7              $S_x \leftarrow (1/4\pi) \times S_0$ 
8
9          $S_D \leftarrow 0$ 
10        for  $E' \in \mathcal{E} | E' \geq E$ 
11             $S_D = S_D + (1/4\pi) \times \phi(r, \Omega, E') \times \Sigma_s(\mathcal{Z}(r), E', E) \times V(r)$ 
12
13         $S_T = S_x + S_D$ 
14        return  $S_T$ 

```

2 Introduction

This document will teach you everything you need to know about the Boltzmann Equation from its derivation to the details of its implementation in computer code.

3 Mathematical Development

3.1 The Boltzmann Equation

The time dependent gamma transport equation can be written as

$$\left[\frac{1}{v(E)} \frac{\partial}{\partial t} + \hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}, E, t) \right] \psi(\mathbf{r}, E, \hat{\Omega}, t) = \int_{4\pi} \int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}, t) \psi(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' + S(\mathbf{r}, E, \hat{\Omega}, t) \quad (3.1.1)$$

However, we are typically not concerned with the transient case in medical diagnostic imaging. We are more interested in the steady state case. The time independent form of Eq. 3.1.1 is written as

$$\left[\hat{\Omega} \cdot \nabla + \Sigma_t(\mathbf{r}, E) \right] \psi(\mathbf{r}, E, \hat{\Omega}) = \int_{4\pi} \int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \psi(\mathbf{r}, E', \hat{\Omega}', t) dE' d\hat{\Omega}' + S(\mathbf{r}, E, \hat{\Omega}) \quad (3.1.2)$$

3.2 Harmonic Approximation

Equation 3.1.2 has a number of terms that cannot be solved directly. Instead, some numerical approximation must be used. The macroscopic scattering cross

section, Σ_s is typically expanded with a Legendre polynomial (for more information of Legendre polynomials, refer to Section 8.2). The expansion is as follows:

$$\Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \approx \sum_{l=0}^L \frac{2l+1}{4\pi} \Sigma_{s,l}(\mathbf{r}, E' \rightarrow E) P_l(\hat{\Omega}' \rightarrow \hat{\Omega}) \quad (3.2.1)$$

where $\Sigma_{s,l}$ is the expansion coefficients termed the "scattering moments." The Legendre polynomials $P_l(\hat{\Omega}' \rightarrow \hat{\Omega})$ are defined as

$$P_l(\hat{\Omega}' \rightarrow \hat{\Omega}) = \frac{1}{2l+1} \sum_{m=-l}^l Y_{l,m}^*(\hat{\Omega}') Y_{l,m}(\hat{\Omega}) \quad (3.2.2)$$

The angular fluence (ϕ) is also expanded as

$$\phi(\mathbf{r}, E', \hat{\Omega}') \approx \sum_{l=0}^L \sum_{m=-l}^l \phi_{lm}(\mathbf{r}, E') Y_{l,m}(\hat{\Omega}') \quad (3.2.3)$$

A source term suitable for numeric integration is then

$$\begin{aligned} \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(\mathbf{r}, E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) \phi(\mathbf{r}, E', \hat{\Omega}') &\approx \\ \sum_{l=0}^L \frac{2l+1}{4\pi} \sum_{m=-l}^l \Sigma_{s,l}^{gg'} \phi_{i,j,k,lm}^{g'} Y_{l,m}(\hat{\Omega}_n) & \end{aligned} \quad (3.2.4)$$

Finally, substituting Eqs. 3.2.4 and 3.2.3 into 3.2.1, we arrive at

$$\begin{aligned} \hat{\Omega}_n \cdot \nabla \psi_{i,j,k,n}^g + \sigma_{i,j,k}^g \psi_{i,j,k,n}^g = \\ \sum_{g'=0}^G \sum_{l=0}^L \frac{2l+1}{4\pi} \sum_{m=-l}^l \sigma_{s,l}^{g,g'} \psi_{i,j,k,l,m}^{g'} Y_{l,m}(\hat{\Omega}_n) + \frac{1}{4\pi} q_{i,j,k}^g & \end{aligned} \quad (3.2.5)$$

We can calculate the scalar flux as

$$\phi_{i,j,k}^g = \sum_{n=1}^{|\Omega|} w_n \psi_{i,j,k,n}^g \quad (3.2.6)$$

3.3 Discretization

The continuous Boltzmann Equation Approximation has to be discretized in all dimensions to run on a computer.

The gradient of ψ is calculated as



Figure 1: Simulation Results

$$\nabla \psi_{i,j,k,n}^g \approx \left\langle \frac{\psi_{i+1,j,k}^g - \psi_{i-1,j,k}^g}{\Delta x}, \frac{\psi_{i,j+1,k}^g - \psi_{i,j-1,k}^g}{\Delta y}, \frac{\psi_{i,j,k+1}^g - \psi_{i,j,k-1}^g}{\Delta z} \right\rangle \quad (3.3.1)$$

There are six faces on each parallelepiped with normals $\langle \pm 1, 0, 0 \rangle$, $\langle 0, \pm 1, 0 \rangle$, and $\langle 0, 0, \pm 1 \rangle$. Taking the dot product of these normals and the evaluated gradient gives

$$\hat{\Omega} \cdot \nabla \psi_{i,j,k}^g \approx 2 \left(\frac{\psi_{i+1,j,k}^g - \psi_{i-1,j,k}^g}{\Delta x} + \frac{\psi_{i,j+1,k}^g - \psi_{i,j-1,k}^g}{\Delta y} + \frac{\psi_{i,j,k+1}^g - \psi_{i,j,k-1}^g}{\Delta z} \right) \quad (3.3.2)$$

4 Implementation

At this point, we have successfully developed an algorithm that can be implemented on a computer. However, there are many challenges in actually implementing this algorithm.

4.1 Design

Yeah, it was designed.

4.2 Language Selection

Yeah, it was selected.

4.3 Salome

We chose to use the Salome framework for numerical pre/post-processing. Salome includes a built in geometry system and meshing capabilities.

4.4 Framework Integration

Yeah, it was integrated

4.5 C++ Implementation

Yeah, it was implemented.

```
1 #include <stdio.h>
2 #define N 10
3 /* Block
4  * comment */
5
6 int main()
7 {
8     int i;
9
10    // Line comment.
11    puts("Hello world!");
12
13    for (i = 0; i < N; i++)
14    {
15        puts("LaTeX is also great for programmers!");
16    }
17
18    return 0;
19 }
```

5 MPI Implementation

MPI stands for Message Passing Interface and is the *de Facto* standard for implementing parallel algorithms across multiple physical machines.

6 GPU Implementation

GPU stands for Graphical Processing Unit and is a collection of SIMD (single instruction multiple data) processors. Each processor operates on its own piece of data but performs the same operation each other processor in its warp is executing.

Table 1: A list of solutions to Laplace's equation in different geometrical systems

Cartesian	Exponential, Circular (a class of trig function), hyperbolic
Cylindrical	Bessel, Exponential, Circular
Spherical	Legendre polynomial, Power, Circular

7 Conclusion

Hooray! It works!

8 Appendix

8.1 Laplace's Equation

Many physical phenomena can be described by Poisson's Equation given below.

$$\nabla^2 f = \psi \quad (8.1.1)$$

Laplace's Equation is a special form of Poisson's Equation and is given by Eq. 8.1.2.

$$\nabla^2 f = 0 \quad (8.1.2)$$

Laplace's equation in cartesian coordinates expands to

$$\nabla^2 f(x, y, z) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} = 0 \quad (8.1.3)$$

In cylindrical coordinates

$$\nabla^2 f(r, \phi, z) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \phi^2} + \frac{\partial^2 f}{\partial z^2} \quad (8.1.4)$$

In spherical coordinates

$$\nabla^2 f(\rho, \theta, \phi) = \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial f}{\partial \rho} \right) + \frac{1}{\rho^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial f}{\partial \theta} \right) + \frac{1}{\rho^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2} \quad (8.1.5)$$

Any solution to Laplace's equation is known as a harmonic function. Further, if any two functions are a solution to Laplace's equation, then by the superposition principle, the summation of the two functions is also a solution to Laplace's equation.

Common solutions to Laplace's equation include

8.2 Legendre Polynomials

Legendre polynomials are solutions to

$$P_n(x) = \frac{1}{2\pi i} \oint (1 - 2\xi x + \xi^2)^{-1/2} \xi^{-n-1} d\xi \quad (8.2.1)$$

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n \quad (8.2.2)$$

The first few such solutions are

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

$$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

$$P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)$$

$$P_6(x) = \frac{1}{16}(231x^6 - 315x^4 + 105x^2 - 5)$$

Associated Legendre polynomials are a generalization of the Legendre polynomial and solve

$$P_l^m(x) = (-1)^m (1 - x^2)^{m/2} \frac{d^m P_l(x)}{dx^m} \quad (8.2.3)$$

Both Legendre polynomials and Associated Legendre Polynomials can be calculated using the Boost C++ library.

8.3 Spherical Harmonic Function

First, we assume that Laplace's equation is of the separable form $f(\rho, \theta, \phi) = R(\rho)Y(\theta, \phi)$. Equation 8.1.5 can then be rewritten as

$$\begin{aligned} \nabla^2 f(\rho, \theta, \phi) &= \frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial(R(\rho)Y(\theta, \phi))}{\partial \rho} \right) + \\ &\quad \frac{1}{\rho^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial(R(\rho)Y(\theta, \phi))}{\partial \theta} \right) + \frac{1}{\rho^2 \sin^2 \theta} \frac{\partial^2(R(\rho)Y(\theta, \phi))}{\partial \phi^2} = 0 \end{aligned} \quad (8.3.1)$$

which simplifies to

$$\begin{aligned} \frac{Y(\theta, \phi)}{\rho^2} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial R(\rho)}{\partial \rho} \right) + \frac{R(\rho)}{\rho^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \\ \frac{R(\rho)}{\rho^2 \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} = 0 \end{aligned} \quad (8.3.2)$$

Multiplying Eq. 8.3.2 by $\rho^2/(R(\rho)Y(\theta, \phi))$ yields

$$\begin{aligned} \frac{1}{R(\rho)} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial R(\rho)}{\partial \rho} \right) + \frac{1}{Y(\theta, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \\ \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} = 0 \end{aligned} \quad (8.3.3)$$

Equation 8.3.3 can be split into two parts, a function of ρ alone and a component that is a function of θ and ϕ alone. The component that is a function of θ and ϕ can be moved to the other side of the equation. Since two functions of different variables are equal, they must each be equal to some constant, λ . Therefore, Eq. 8.3.3 can be rewritten as two equations:

$$\frac{1}{R(\rho)} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial R(\rho)}{\partial \rho} \right) = \lambda \quad (8.3.4)$$

$$\frac{1}{Y(\theta, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{Y(\theta, \phi) \sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} = -\lambda \quad (8.3.5)$$

$Y(\theta, \phi)$ can be further separated into $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$ which produces

$$\begin{aligned} \frac{1}{\Theta(\theta)\Phi(\phi) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial(\Theta(\theta)\Phi(\phi))}{\partial \theta} \right) + \\ \frac{1}{\Theta(\theta)\Phi(\phi) \sin^2 \theta} \frac{\partial^2(\Theta(\theta)\Phi(\phi))}{\partial \phi^2} = -\lambda \end{aligned} \quad (8.3.6)$$

which simplifies to

$$\frac{1}{\Theta(\theta) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} \right) + \frac{1}{\Phi(\phi) \sin^2 \theta} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} = -\lambda \quad (8.3.7)$$

Multiplying Eq. 8.3.7 by $\sin^2(\theta)$ and rearranging yields

$$\frac{\sin \theta}{\Theta(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} \right) + \lambda \sin \theta = \frac{-1}{\Phi(\phi)} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} \quad (8.3.8)$$

As before, each side of Eq. 8.3.8 is a function of a single variable, therefore, both sides are equal to some constant. In this case, we select m^2 to be the constant variable. This produces

$$\frac{\sin \theta}{\Theta(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} \right) + \lambda \sin \theta = m^2 \quad (8.3.9)$$

$$\frac{1}{\Phi(\phi)} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} = -m^2 \quad (8.3.10)$$

Combining Eq. 8.3.4, 8.3.9, and 8.3.10 Laplace's equation in spherical coordinates can be expressed in a fully separated form as

$$\begin{aligned} \frac{1}{R(\rho)} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial R(\rho)}{\partial \rho} \right) &= \lambda \\ \frac{\sin \theta}{\Theta(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} \right) + \lambda \sin \theta &= m^2 \\ \frac{1}{\Phi(\phi)} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} &= -m^2 \end{aligned} \quad (8.3.11)$$

It can be shown through a detailed analysis that is outside the scope of this paper that m and λ must both be integers. λ is further constrained in that the relation $\lambda = l(l+1)$ where $l \leq |m|$ and $l \in \mathbb{Z}$. Therefore, Eq. 8.3.11 can be written as

$$\begin{aligned} \frac{1}{R(\rho)} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial R(\rho)}{\partial \rho} \right) &= l(l+1) \\ \frac{\sin \theta}{\Theta(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} \right) + l(l+1) \sin \theta &= m^2 \\ \frac{1}{\Phi(\phi)} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} &= -m^2 \\ l, m \in \mathbb{Z} \\ l \leq |m| \end{aligned} \quad (8.3.12)$$

TODO - Discontinuous

It can be shown that the solution is stated

$$Y_l^m(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} \frac{(l-m)!}{(l+m)!} P_l^m(\cos \theta) e^{im\phi} \quad (8.3.13)$$

whose real part can be expanded to

$$Y_l^0 = \sqrt{\frac{2l+1}{4\pi}} P_l^0(1) \quad (8.3.14)$$

$$Y_l^{m,even} = (-1)^m \sqrt{\frac{2l+1}{2\pi}} \frac{(l-m)!}{(l+m)!} P_l^m(\cos(m\phi)) \quad (8.3.15)$$

$$Y_l^{m,odd} = (-1)^m \sqrt{\frac{2l+1}{2\pi}} \frac{(l-m)!}{(l+m)!} P_l^m(\sin(m\phi)) \quad (8.3.16)$$

8.4 Klein-Nishina Formula

The Klein-Nishina formula gives the differential scattering cross section of photon incident on a single free electron.

$$\frac{\partial\sigma}{\partial\Omega} = \frac{1}{2}\alpha^2 r_c^2 P(E_\gamma, \theta)^2 (P(E_\gamma, \theta) + P(E_\gamma, \theta)^{-1} - 1 + \cos^2(\theta)) \quad (8.4.1)$$

$$P(E_\gamma, \theta) = \frac{1}{1 + (\frac{E_\gamma}{m_e c^2})(1 - \cos(\theta))} \quad (8.4.2)$$

where α is the fine structure constant ($\alpha \approx 7.2971E - 3$), r_c is the reduced Compton wavelength ($r_c = \hbar$)

8.5 Numeric Integration

$$\tilde{H} \quad (8.5.1)$$