Energy-dependent analytical solutions for the charged particle transport equation

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ICTT-22, Portland, Oregon
September 15, 2011
Overview

- Background
- Derivation of analytical results
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The Boltzmann equation under CSDA

Under the continuous slowing down assumption (CSDA), the stationary Boltzmann equation for the fluence $f$ of charged particles with energy $E$ traveling in direction $\Omega \in S^2$, given an incident particle beam into the half-space $z \geq 0$, is

$$
\begin{align*}
\Omega \cdot \nabla f(x, E, \Omega) + \sigma_a(E)f(x, E, \Omega) - \frac{\partial (S(E)f)}{\partial E} - \frac{1}{2} \frac{\partial^2 (\omega(E)f)}{\partial E^2} &= \\
\int_{S^2} \sigma_s(E, \Omega \cdot \Omega')(f(x, E, \Omega') - f(x, E, \Omega)) \, d\Omega' \\
f|_{z=0} &= f_0(x, y, \Omega)G(E)
\end{align*}
$$

Here, $\sigma_a(E)$ is the absorption cross-section, while $\sigma_s(E, \Omega \cdot \Omega')$ is the scattering cross-section. $S(E)$ is the stopping power, and $\omega(E)$ is the energy-loss straggling coefficient.
The Fermi-Eyges equation (1)

Enrico Fermi suggested the equation below for narrow beams in the late 30's (Rossi and Greisen, 1941). Eyges (1948) extended it to $T = T(z)$ and derived an analytical solution when $f_0(x, y, \theta_x, \theta_y) = \delta(x)\delta(y)\delta(\theta_x)\delta(\theta_y)$.

$$\frac{\partial \psi}{\partial z} + \theta_x \frac{\partial \psi}{\partial x} + \theta_y \frac{\partial \psi}{\partial y} = \frac{T(z)}{2} \left( \frac{\partial^2 \psi}{\partial \theta_x^2} + \frac{\partial^2 \psi}{\partial \theta_y^2} \right)$$

(2)

It can be viewed as the projection of the Fokker-Planck equation onto the tangent plane at $\Omega = [0, 0, 1]$ (Börgers and Larsen, 1996).
The Fermi-Eyges equation (2)

The analytical solution for an incident Gaussian beam $G_1(x, y, \theta_x, \theta_y)$ is (Brahme, 1975):

$$h_{FE}(x, y, z, \theta_x, \theta_y) = C(z) \exp \left( -a(z)(x^2 + y^2) - 2b(z)(x\theta_x + y\theta_y) - c(z)(\theta_x^2 + \theta_y^2) \right), \quad (3)$$

where $a(z)$, $b(z)$, $c(z)$ and $C(z)$ may be computed explicitly from the first three moments of $T(z)$ (formulas omitted here).
Derivation of energy dependence

Using the Fermi-Eyges approximation for the scattering term, and the CSDA assumption for energy dependence, we get the equation

\[
\begin{aligned}
\frac{\partial f}{\partial z} + \theta_x \frac{\partial f}{\partial x} + \theta_y \frac{\partial f}{\partial y} + \sigma_a(E) f - \frac{\partial}{\partial E} (S(E)f) - \frac{1}{2} \frac{\partial^2}{\partial E^2} (\omega(E)f) \\
= T(z) \left( \frac{\partial^2 f}{\partial \theta_x^2} + \frac{\partial^2 f}{\partial \theta_y^2} \right),
\end{aligned}
\]

(4)

where

\[
T(z) = \int_{-1}^{1} \sigma_s(\bar{E}(z), \mu) \cdot \mu^2 d\mu
\]

(5)

and \(\bar{E}(z)\) is the average energy at depth \(z\) (which is not yet determined). Equation (4) is **separable** and we will now use this fact to derive analytical solutions.
No straggling (1)

In the case when the straggling term is ignored \( \omega(E) \equiv 0 \), the ansatz

\[
f(r, \theta_x, \theta_y, E) = g(E)h(r, \theta_x, \theta_y).
\] (6)

yields the two equations

\[
\frac{\partial}{\partial E} \left( S(E)g(E) \right) - \sigma_a(E)g(E) = \lambda g(E) \] (7)

\[
\frac{\partial h}{\partial z} + \theta_x \frac{\partial h}{\partial x} + \theta_y \frac{\partial h}{\partial y} - T(z) \left( \frac{\partial^2 h}{\partial \theta_x^2} + \frac{\partial^2 h}{\partial \theta_y^2} \right) = \lambda h(r, \theta_x, \theta_y),
\] (8)

for some constant \( \lambda \). These can now be solved separately. Equation (7) is solved using an integrating factor to yield

\[
g(E) = g(E_0) \frac{S(E_0)}{S(E)} \exp \left( \lambda (R(E) - R(E_0)) - \int_{E_0}^E \frac{\sigma_a(E')}{S(E')} dE' \right),
\] (9)

where \( R(E) = \int_0^E \frac{dE'}{S(E')} \) is the CSDA range.

Equation (8) is the Fermi-Eyges equation with a right-hand side and has the solution

\[
h(r, \theta_x, \theta_y) = e^{\lambda z} h_{FE}(r, \theta_x, \theta_y),
\] (10)

where \( h_{FE} \) is the Fermi-Eyges solution.
No straggling (2)

Combining the two solutions, and introducing the relationship

\[ z(E) = R(E_0) - R(E), \tag{11} \]

or equivalently, \( E = \bar{E}(z) \), to satisfy the boundary condition (4) with \( G_2(E) = \delta(E - E_0) \) and get a single energy at each depth, the dependence on \( \lambda \) disappears and

\[
f(r, \theta_x, \theta_y) = \frac{S(E_0)}{S(E(z))} \exp \left( - \int_{E(z)}^{E_0} \frac{\sigma_a(E')}{S(E')} \, dE' \right) h_{FE}(r, \theta_x, \theta_y). \tag{12} \]

is a solution to (4) with \( \omega(E) \equiv 0 \) for mono-energetic particle beams.

NB: This solution was suggested by (Kempe and Brahme, 2010) without rigorous derivation.
With energy-loss straggling

When we include the straggling term \( \omega(E) > 0 \), we make a more general ansatz:

\[
f(r, \theta_x, \theta_y, E) = h_{FE}(r, \theta_x, \theta_y) \cdot Z(z, E) \neq 0.
\]  

(13)

With this ansatz, equation (4) yields

\[
\gamma_{FE}[h_{FE}] \cdot Z + h_{FE} \left( \frac{\partial Z}{\partial z} - \frac{\partial (S(E)Z)}{\partial E} - \frac{1}{2} \frac{\partial^2 (\omega(E)Z)}{\partial E^2} + \sigma_a(E)Z \right) = 0,
\]  

(14)

where \( \gamma_{FE}[h_{FE}] \) stands for the Fermi-Eyges equation and is identically zero for the solution \( h_{FE} \).

Therefore, we get the following equation for \( Z(z, E) \)

\[
\begin{cases}
\frac{\partial Z}{\partial z} - \frac{\partial (SZ)}{\partial E} - \frac{1}{2} \frac{\partial^2 (\omega Z)}{\partial E^2} + \sigma_a(E)Z = 0, & (z, E) \in [0, \infty) \times [0, \infty), \\
Z(0, E) = G_2(E), & E \geq 0, \\
Z(z, 0) = 0, & z \geq 0
\end{cases}
\]  

(15)
Analytical result with NESA

In order to get an analytical solution, we wish to apply the Fourier transform in $E$, and therefore wish to extend the problem to $E \in \mathbb{R}$. In order to retain the boundary condition $Z(z, 0) = 0$, we look for solutions $Z$ that are odd in $E$, so that $Z(z, -E) = -Z(z, E), z \geq 0$.

Furthermore, we invoke the narrow energy spectrum approximation (NESA), i.e.

$$\mathcal{F}(w(E) \cdot Z(E)) \approx w(\bar{E}(z)) \cdot \hat{Z}(z, \xi).$$  \hspace{1cm} (16)$$

Solving the resulting equation in the Fourier domain yields the result

$$Z(z, E) = \frac{C_0}{\sqrt{2\pi \Omega(z)}} \exp(-\Sigma_a(z)) \left( \exp\left(-\frac{1}{2} \frac{(E - \bar{E}(z))^2}{\Omega(z)}\right) \right.$$  \hspace{1cm} (17)

$$\left. - \exp\left(-\frac{1}{2} \frac{(E + \bar{E}(z))^2}{\Omega(z)}\right) \right),$$

where

$$\Sigma_a(z) = \int_0^z \sigma_a(\bar{E}(z')) \, dz', \hspace{1cm} \bar{E}(z) = E_0 - \int_0^z S(\bar{E}(z')) \, dz',$$

$$\Omega(z) = \Omega_0 + \int_0^z \omega(\bar{E}(z')) \, dz'.$$  \hspace{1cm} (18)
Analytical result with NESA (2)

Note that (17) satisfies the boundary condition in (4) with

\[ G_2(E) = \frac{C_0}{\sqrt{2\pi}\Omega_0} \left( \exp \left( -\frac{1}{2} \frac{(E - E_0)^2}{\Omega_0} \right) - \exp \left( -\frac{1}{2} \frac{(E + E_0)^2}{\Omega_0} \right) \right), \] (19)

that is, a Gaussian energy distribution for \( E > 0 \) if \( \Omega_0 \) is small enough so that the mirrored part has negligible influence for \( E > 0 \).
In order to investigate the accuracy of the NESA we have performed numerical computations for equation (15) using the finite element method. We treated $z$ as a time variable with a backward Euler scheme, and with piece-wise linear (CG1) elements in $E$. A $800 \times 800$ non-uniform grid was used. Cross-sections for electrons in water were taken from (Luo and Brahme, 1992). Parameters used:

1. $E_0 = 50$ MeV, $\Omega_0 = 4.4$ MeV$^2$, $C_0 = \sqrt{2\pi\Omega_0}$,
2. $E_0 = 20$ MeV, $\Omega_0 = 0.7$ MeV$^2$, $C_0 = \sqrt{2\pi\Omega_0}$,
Comparison - results (1)

Figure: Level curves for the numerical solution to equation (15) (left), and the analytical solution (17) under the narrow energy spectrum approximation (NESA) (right). The incident beam has mean energy $E_0 = 50$ MeV. The cross-sections for electrons in water were used. The dashed lines are the curves $E = \bar{E}(z)$, and the red lines are the averages energies for the respective solutions.
Comparison - results (2)

Figure: Level curves for the numerical solution to equation (15) (left), and the analytical solution (17) under the narrow energy spectrum approximation (NESA) (right). The incident beam has mean energy $E_0 = 20$ MeV. The cross-sections for electrons in water were used. The dashed lines are the curves $E = \bar{E}(z)$, and the red lines are the averages energies for the respective solutions.
Summary/conclusion

- We have derived energy-dependent analytical solutions for the Fermi-Eyges equation under a continuous slowing down assumption.
- In the straggling case, the NESA was used to obtain an analytical solution.
- Analytical solutions were compared to numerical results using the Finite Element Method, showing reasonable agreement.
Acknowledgments

- Anders Brahme, Karolinska Institute
- Luo Zhengming for inspiration
Thank you!
References


