IOP Publishing | Institute of Physics and Engineering in Medicine   Physics in Medicine & Biology

Phys. Med. Biol. **60** (2015) 4963–4971   doi:10.1088/0031-9155/60/13/4963

Lorentz force correction to the Boltzmann radiation transport equation and its implications for Monte Carlo algorithms

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Received 26 July 2014, revised 22 September 2014
Accepted for publication 9 October 2014
Published 10 June 2015

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Abstract

To establish a theoretical framework for generalizing Monte Carlo transport algorithms by adding external electromagnetic fields to the Boltzmann radiation transport equation in a rigorous and consistent fashion. Using first principles, the Boltzmann radiation transport equation is modified by adding a term describing the variation of the particle distribution due to the Lorentz force. The implications of this new equation are evaluated by investigating the validity of Fano's theorem. Additionally, Lewis' approach to multiple scattering theory in infinite homogeneous media is redefined to account for the presence of external electromagnetic fields. The equation is modified and yields a description consistent with the deterministic laws of motion as well as probabilistic methods of solution. The time-independent Boltzmann radiation transport equation is generalized to account for the electromagnetic forces in an additional operator similar to the interaction term. Fano's and Lewis' approaches are stated in this new equation. Fano's theorem is found not to apply in the presence of electromagnetic fields. Lewis' theory for electron multiple scattering and moments, accounting for the coupling between the Lorentz force and multiple elastic scattering, is found. However, further investigation is required to develop useful algorithms for Monte Carlo and deterministic transport methods. To test the accuracy of Monte Carlo transport algorithms in the presence of electromagnetic fields, the Fano cavity test, as currently defined, cannot be applied. Therefore, new tests must be designed for this specific application. A multiple scattering theory that accurately couples the Lorentz force with elastic scattering could improve Monte Carlo efficiency. The present study proposes a new theoretical framework to develop such algorithms.

Keywords: electron/positron Monte Carlo transport methods, external electromagnetic forces, Boltzmann transport equation, Fano theorem, Lewis theory

(Some figures may appear in colour only in the online journal)

1. Introduction

The integration of magnetic resonance imaging (MRI) and radiotherapy (RT) promises great advantages for image guidance during treatment. This could yield major benefits in terms of dose delivery accuracy through high-contrast and real-time imaging without exposing patients to unnecessary radiation. However, it has been reported that MRI-strength magnetic fields (i.e. 0.2 T or more) can have significant effects on radiation dosimetry (Nath and Schulz 1978, Bielajew 1993, Nardi and Barnea 1999, Reiffel *et al* 2000, Li *et al* 2001, Raaymakers *et al* 2004, Raaijmakers *et al* 2005, Raaijmakers *et al* 2007, Kirkby *et al* 2008, Meijsing *et al* 2009, Reynolds *et al* 2013). These effects must be modeled using Monte Carlo (MC) codes that combine deterministic Lorentz forces with stochastic interactions. At present, these interactions are treated typically as independent processes (Bielajew 1989, Bielajew 2001, Jette 2000, Agostinelli *et al* 2003, Salvat *et al* 2009, Yang and Bednarz 2013). In reality, the multiple scattering (MS) of charged particles and the Lorentz forces are coupled to the charged particles' directions and the assumption of the independence of these processes can bias the results. This error can be reduced using small steps sizes, at the expense of reduced computational efficiency. Furthermore, apart from a direct comparison with time-consuming single-scattering mode simulations, such an implementation lacks rigorous self-consistency validation methods. This is because it has not been shown that the conditions required by the Fano cavity test (Bielajew 1990a, 1990b, Kawrakow 2000a, Sempau and Andreo 2006, Sterpin *et al* 2013) in varying density media, can be achieved in the presence of electromagnetic (EM) fields. Herein, we propose a new theoretical framework that couples EM fields to radiation transport and suggest two new algorithms for MC calculations.

In this work, the Boltzmann transport equation for electrons and positrons is modified to account for the deterministic effects of Lorentz forces and the applicability of Fano's theorem (Fano 1954) using EM fields is investigated. Using the same approach as in Lewis' theory (Lewis 1950), the transport equations can be cast into a spherical harmonics expansion framework to investigate the feasibility of developing a new algorithm that takes into account, the coupling between MS and EM fields.

2. Theory

2.1. Definitions

Let us define the following:

- $\vec{r}$: a vector corresponding to the particle's position in space
- $\vec{p}$: a vector corresponding to the particle's momentum
- $\vec{u}$: a unit vector in the same direction as $\vec{p}$
- β: the particle's velocity relative to c
- t: time
- s: the path traversed by the particle between time 0 and t
- $n(\vec{r}, \vec{p}, t)$: the spatial particle distribution at time t corresponding to the number of particles with momentum $\vec{p}$ per unit volume dV, unit momentum dp and per unit solid angle of particle direction $\sin\theta \, \mathrm{d}\theta \, \mathrm{d}\phi$

- $f(\vec{r},\vec{p},t)$: the particle flux corresponding at time t to the number of particles with momentum $\vec{p}$ per unit area dA perpendicular to the particle direction, unit momentum dp and per unit solid angle of particle direction $\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$.

2.2. Radiation transport equation

For each particle type, a transport equation can be written in generality, as follows. One starts from the continuity equation and adds the source and collision terms on the right-hand side:

$$\frac{\mathrm{d}n}{\mathrm{d}t} = \rho\,[S + I]\,, \tag{1}$$

where $n = n(\vec{r},\vec{p},t)$ and $\rho = \rho(\vec{r})$, the mass density. Here, $S = S(\vec{r},\vec{p},t)$ is the source term and represents the differential number of particles being generated with given momentum per unit mass and unit time, by an external source at a given position in space. The term I, is the interaction term representing the differential number of particles being generated with given momentum per unit mass and unit time through collisions at a given position in space. The interaction term is represented by an integral-differential operator on the flux f and is a function of the physical properties of the media, i.e. $I = I\,\{f;\vec{r}\}$.

3. Methods

3.1. Decomposition into multi-variable dependencies

For a given momentum $\vec{p}$, one can write

$$\begin{aligned}\frac{\mathrm{d}n}{\mathrm{d}t} &= \frac{\partial n}{\partial t} + \frac{\partial n}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial n}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t} + \frac{\partial n}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t} + \frac{\partial n}{\partial p_x}\frac{\mathrm{d}p_x}{\mathrm{d}t} + \frac{\partial n}{\partial p_y}\frac{\mathrm{d}p_y}{\mathrm{d}t} + \frac{\partial n}{\partial p_z}\frac{\mathrm{d}p_z}{\mathrm{d}t}\\ &= \frac{\partial n}{\partial t} + \frac{\mathrm{d}\vec{r}}{\mathrm{d}t}\cdot\vec{\nabla}_r\,n + \frac{\mathrm{d}\vec{p}}{\mathrm{d}t}\cdot\vec{\nabla}_p\,n\,.\end{aligned} \tag{2}$$

Since the particle distribution and flux are linked by the following equation

$$f = n\beta c, \tag{3}$$

one writes

$$\frac{\mathrm{d}n}{\mathrm{d}t} = \frac{1}{\beta c}\frac{\partial f}{\partial t} + \vec{u}\cdot\vec{\nabla}_r f + \frac{\mathrm{d}\vec{p}}{\mathrm{d}t}\cdot\left[\frac{1}{\beta c}\,\vec{\nabla}_p f + \frac{1}{c} f\,\vec{\nabla}_p\,\frac{1}{\beta}\right]. \tag{4}$$

where the property d$s = \beta\,c$dt is used. Since $p = \gamma\beta\,mc$, one can write

$$\beta = \sqrt{\frac{\left(\frac{p}{mc}\right)^2}{1 + \left(\frac{p}{mc}\right)^2}}$$

and using the spherical coordinates of $\vec{p}$ one obtains

$$
\begin{aligned}
\vec{\nabla}_p \frac{1}{\beta} &= \vec{u}\frac{\partial}{\partial p}\sqrt{\frac{1}{\left(\frac{p}{mc}\right)^2}+1} \\
&= -\vec{u}\frac{1}{\sqrt{\frac{1}{\left(\frac{p}{mc}\right)^2}+1}}\frac{1}{\left(\frac{p}{mc}\right)^3}\frac{1}{mc} \\
&= -\frac{1}{\gamma^3\beta^2 mc}\vec{u}.
\end{aligned} \tag{5}
$$

Combining equations (1), (4) and (5), the following relation is obtained:

$$
\frac{1}{\beta c}\frac{\partial f}{\partial t}+\vec{u}\cdot\vec{\nabla}_r f+\frac{\mathrm{d}\vec{p}}{\mathrm{d}t}\cdot\left[\frac{1}{\beta c}\vec{\nabla}_p f-\frac{1}{\gamma^3\beta^2 mc}f\vec{u}\right]=\rho\,[S+I]\,. \tag{6}
$$

3.2. The Lorentz force

The Lorentz force describes the deterministic momentum variation of a charged particle in the presence of electric, $\vec{E}$ and magnetic, $\vec{B}$, fields. The deterministic equation of motion is written as

$$
\left[\frac{\mathrm{d}\vec{p}}{\mathrm{d}t}\right]_{\text{Lorentz}}=q\,[\vec{E}+\beta c\vec{u}\times\vec{B}]\,. \tag{7}
$$

It is worth defining the Lorentz force term as the following position-dependent operators

$$
\begin{aligned}
F_{\text{Lorentz}}\{f;\vec{E},\vec{B}\} &\equiv -q\,[\vec{E}+\beta c\vec{u}\times\vec{B}]\cdot\left[\frac{1}{\beta c}\vec{\nabla}_p f-\frac{1}{\gamma^3\beta^2 mc}f\vec{u}\right] \\
&= -q\left[\frac{\vec{E}}{\beta c}+\vec{u}\times\vec{B}\right]\cdot\vec{\nabla}_p f+\frac{q}{\gamma^3\beta^2 mc}\,[\vec{E}\cdot\vec{u}]\,f.
\end{aligned} \tag{8}
$$

Note here the implicit spatial dependencies $\vec{E}=\vec{E}(\vec{r})$ and $\vec{B}=\vec{B}(\vec{r})$ being expressed in the operator F_{Lorentz}. In the presence of the external fields $\vec{E}$ and $\vec{B}$, the time-dependent transport equation becomes

$$
\frac{\partial f}{\partial s}+\vec{u}\cdot\vec{\nabla}_r f=\rho\,[S(\vec{r},\vec{p},t)+I\{f;\vec{r}\}\,]+F_{\text{Lorentz}}\{f;\vec{E},\vec{B}\}\,, \tag{9}
$$

with s the particle path whose differential is defined as $\mathrm{d}s=\beta\,c\mathrm{d}t$.

3.3. Time-independent transport equation

It is worth looking at the situation where the external fields $\vec{E}$ and $\vec{B}$ are constant over time and where either the source is constant over time (equilibrium state), or the flux is integrated over time (fluence). With a few simplifications, the time-independent equation can be written

$$
\vec{u}\cdot\vec{\nabla}_r f=\rho\,[S(\vec{r},\vec{p})+I\{f;\vec{r}\}\,]+F_{\text{Lorentz}}\{f;\vec{E},\vec{B}\}\,. \tag{10}
$$

4. Applications and results

4.1. Non applicability of Fano's theorem in the presence of electromagnetic fields

The result of Fano's theorem (Fano 1954) has been exploited to benchmark charged particle transport of Monte Carlo codes (Kawrakow 2000a, Sempau and Andreo 2006, Sterpin *et al* 2013, Poon and Verhaegen 2005). The rationale of this approach, also known as the *Fano cavity test*, is based on artificially creating charged particle equilibrium (CPE), in a medium of uniform properties allowing one to obtain an analytic expression to calculate the absorbed dose. One consequence of the theorem for photon beams is that the absorbed dose equals collision kerma independently of the mass density distribution within the geometry. This analytic solution is then compared to the simulation results in order to evaluate the self-consistency of the charged particle transport algorithm within its own cross-sections.

The Fano theorem's derivation, starting with the transport equation, is relatively straight forward. In the absence of external EM fields, the left-hand side of equation (10) describing charged particles, vanishes when the flux (or fluence) is constant ($\vec{u}\cdot\vec{\nabla}_r f = 0$). This condition of uniform flux (or fluence), is also known as CPE. Since the right-hand side of the equation is proportional to the mass density, it may be cancelled out and the solution of the transport equation is, therefore, independent of mass density. A Monte Carlo simulation using a uniform charged particle source per unit mass and a geometry having uniform interaction cross sections, has the consequence of generating the same fluence, for a given source per unit mass, independently of the mass density distribution.

When external EM fields are present, the same approach does not yield the same result. Using equation (10) and stating the condition of CPE, one writes

$$\rho\,[S(\vec{r},\vec{p}) + I\{f;\vec{r}\}\,] - q\left[\frac{\vec{E}}{\beta c} + \vec{u}\times\vec{B}\right]\cdot\vec{\nabla}_p f + \frac{q}{\gamma^3\beta^2 mc}\,[\vec{E}\cdot\vec{u}]\,f \overset{\text{CPE}}{=} 0. \qquad (11)$$

One can clearly observe that for Fano's theorem to be valid, the norms of the vector fields $\vec{E}$ and $\vec{B}$ must be proportional to mass density. Although the medium permittivity and permeability can affect the strength of the fields with respect to the same strengths in vacuum, in general EM fields do not scale with mass density. Therefore, Fano's theorem cannot be valid in the presence of such external fields.

4.2. Modification of Lewis' approach to multiple scattering theory

Multiple scattering (MS) theory is at the core of condensed history (CH) algorithms (Berger 1963) used to simulate the transport of charged particle in matter. The rationale behind the approach is to combine single elastic scattering events, occurring between the particle in motion and atomic nuclei, into single virtual interactions along the particle track in order to save significant computation time.

While several approaches to MS are found in the literature (Goudsmit and Saunderson 1940, Rossi and Greisen 1941, Eyges 1948, Lewis 1950, Bethe 1953, Larsen 1992, Kawrakow and Bielajew 1998a, Kawrakow 2000b), Lewis' (1950) theory is the most general and exact. The rationale behind the idea is to solve the statistical moments of the particle distribution after a step of given length in an infinite homogeneous medium, independently of the scattering model used. In contrast to other approaches which provide a probability density function, e.g. the small-angle approximation of Moliere (Bethe 1953), Lewis' moments can be used to benchmark MS algorithms in order to evaluate their accuracy (Kawrakow and Bielajew 1998b).

To validate the coupling of EM fields to CH algorithms, Lewis' approach can be modified by integrating the deterministic effect of the Lorentz force into the transport equation. The problem is approached under two conditions. One is the case where $\vec{E} = \vec{0}$ and can be solved considering energy loss implicitly using the continuous slowing down approximation (CSDA). In such approximation, the momentum p can be entirely determined by s since $\vec{B}$ does not change the energy of charged particles. This allows the modified transport equation to be written as

$$\begin{aligned}\frac{\partial f(\vec{r},\vec{u},s)}{\partial s} + \vec{u}\cdot\vec{\nabla}_r f(\vec{r},\vec{u},s) = N\int_{4\pi}&[f(\vec{r},\vec{u}\,',s) - f(\vec{r},\vec{u},s)]\;\sigma(p(s),\vec{u}\cdot\vec{u}\,')\mathrm{d}\vec{u}\,' \\ &- q\vec{u}\times\vec{B}\cdot\vec{\nabla}_p f(\vec{r},\vec{u},s),\end{aligned} \tag{12}$$

with N being the number of scattering centres per unit volume.

The second case that must be considered is where $\vec{E} \neq \vec{0}$. Using the CSDA, the deterministic force related to energy loss through collisions can be written as

$$\begin{aligned}\left[\frac{\mathrm{d}\vec{p}}{\mathrm{d}t}\right]_{\mathrm{CSDA}} &= \left[\frac{\mathrm{d}p}{\mathrm{d}t}\right]_{\mathrm{CSDA}}\vec{u} \\ &= \left[\frac{\mathrm{d}\left(\sqrt{E^2 - m^2c^4}\right)}{c\mathrm{d}t}\right]_{\mathrm{CSDA}}\vec{u} \\ &= \left[\frac{E}{\sqrt{E^2 - m^2c^4}}\frac{\mathrm{d}E}{c\mathrm{d}t}\right]_{\mathrm{CSDA}}\vec{u} \\ &= \left[\frac{\gamma mc^2}{pc}\frac{\mathrm{d}E}{c\mathrm{d}t}\right]_{\mathrm{CSDA}}\vec{u} \\ &= \left[\frac{\mathrm{d}E}{\beta c\mathrm{d}t}\right]_{\mathrm{CSDA}}\vec{u} \\ &= -L_\Delta(T)\vec{u},\end{aligned} \tag{13}$$

where $L_\Delta(T)$ is the restricted stopping power as a function of kinetic energy T. The threshold parameter, Δ, is the lower limit for producing secondary particle flux, while $T/2$ is the upper limit (ignoring binding energies). Note here that the restricted stopping power is used in CH algorithms (instead of unrestricted) since charged particle interactions involving energy transfers above Δ are treated analogously (Berger 1963). It is worth defining the CSDA force term as the following position-dependent operators:

$$\begin{aligned}F_{\mathrm{CSDA}}\{f;\vec{r}\} &\equiv L_\Delta(T)\vec{u}\cdot\left[\frac{1}{\beta c}\vec{\nabla}_p f - \frac{1}{\gamma^3\beta^2 mc}f\vec{u}\right] \\ &= \frac{L_\Delta(T)}{\beta c}\frac{\partial f}{\partial p} - \frac{L_\Delta(T)}{\gamma^3\beta^2 mc}f.\end{aligned} \tag{14}$$

Since forces are additive, the force terms are also additive and one writes

$$\frac{\partial f(\vec{r},\vec{p},s)}{\partial s}+\vec{u}\cdot\vec{\nabla}_r f(\vec{r},\vec{p},s)=N\int_{4\pi}[f(\vec{r},\vec{p}\,',s)-f(\vec{r},\vec{p},s)\,]\,\sigma(p,\vec{u}\cdot\vec{u}\,')\,\mathrm{d}\vec{u}\,'$$
$$-q\left[\frac{\vec{E}}{\beta c}+\vec{u}\times\vec{B}\right]\cdot\vec{\nabla}_p f(\vec{r},\vec{p},s)+\frac{q}{\gamma^3\beta^2 mc}[\vec{E}\cdot\vec{u}]\,f(\vec{r},\vec{p},s)$$
$$+\frac{L_\Delta(T)}{\beta c}\frac{\partial f(\vec{r},\vec{p},s)}{\partial p}-\frac{L_\Delta(T)}{\gamma^3\beta^2 mc}f(\vec{r},\vec{p},s)\,. \tag{15}$$

To generalize Lewis' approach in the presence of EM fields, statistical moments of the flux distribution f should be evaluated from either equations (12) or (15), depending whether or not $\vec{E}=\vec{0}$. The approach involves expending f into spherical harmonics and solving the moments $<x>$, $<x\cos\theta>$, etc.

5. Discussion

5.1. Fano cavity test in the presence of EM fields

One important result of the present work is the formal proof that Fano's theorem does not hold in the presence of static and constant external EM fields. This has the unfortunate consequence of invalidating the Fano cavity test as it is currently performed to benchmark CH algorithms. Although validating the convergence of such algorithms against single-scattering mode simulations can be assumed to be a sufficient substitution, adapting the Fano cavity test for the presence of EM fields yields additional benefits, such as efficient testing and rigorous comparison with an analytic result. Indeed, performing self-consistency testing of Monte Carlo algorithms against an analytic prediction is incontestably ideal and therefore preserving the value of such a test would be a remarkable benefit. While obtaining an analytic expression of either the electron fluence or the absorbed dose under such conditions could be challenging, further investigation is necessary to design an appropriate test in the presence of EM fields.

5.2. Multiple scattering theory coupled to EM fields

To accurately couple MS and EM fields, stochastic changes in particle velocity due to scattering must be accounted for in the calculation of deterministic trajectories subject to Lorentz force. As a result of the present study, we suggest that Lewis' approach to MS theory can be adapted to the presence of EM fields. It has the major advantage of not requiring the azimuthal symmetry of conventional MS theories, being violated by the deterministic effects of EM fields. The introduction of the Lorentz force in Boltzmann transport equation, as shown in equation (9), yields two conditions: (1) the absence of an electric field, as described by equation (12), that does not necessitate explicit treatment of the energy loss and (2) the presence of an electric field being described by equation (15) that requires explicit treatment of energy loss. Calculating the Lewis moments adapted for EM fields, could potentially lead to the development of a new MS theory that would allow MC transport algorithms to take larger steps without compromising accuracy. Indeed, despite that the efficiency of such algorithms rely on their mathematical strategies, a comparison with Lewis' theory remains unavoidable due to the valuable generality of his approach.

6. Conclusion

By introducing the Lorentz force into the Boltzmann transport equation, the present paper proposes a theoretical framework for developing algorithms relevant to MC transport coupled to EM fields. Firstly, we demonstrate that Fano's theorem does not apply in the presence of EM fields. The main consequence is that the standard Fano cavity test cannot be used with varying mass density media in the presence of EM fields. As a result, a new test must be designed to validate the accuracy of charged particle transport simulation under such conditions. Secondly, we demonstrate that the new Boltzmann equation can be used to develop an exact MS theory, one that allows larger step-sizes, thereby improving simulation efficiency. However, this development breaks the azimuthal symmetry of conventional MS theories, necessitating the development of new techniques. The theoretical framework proposed herein will enable the development of a new accuracy test for MC simulations to assess the influence of EM fields. Additionally, the proposed approach will allow the development of a new MS theory, adapted in a theoretically rigorous fashion, for EM fields, allowing the possibility of a new, highly efficient MC algorithm.

Acknowledgments

One of us (AFB) gratefully acknowledges the hospitality of the Ionizing Radiation Standards Group, at the Institute for National Measurement Standards, National Research Council of Canada, Ottawa, during his sabbatical leave, during which his contribution to this work was performed. We would also like to thank H Palmans and S Duane from NPL for fruitful discussions on the subject.

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