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# A closed-form solution for the two-dimensional transport equation by the $LTS_N$ nodal method in the energy range of Compton effect

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## ABSTRACT

In the present work we report on a closed-form solution for the two-dimensional Compton transport equation by the  $LTS_N$  nodal method in the energy range of Compton effect. The solution is determined using the  $LTS_N$  nodal approach for homogeneous and heterogeneous rectangular domains, assuming the Klein-Nishina scattering kernel and a multi-group model. The solution is obtained by two one-dimensional S<sub>N</sub> equation systems resulting from integrating out one of the orthogonal variables of the  $S_N$  equations in the rectangular domain. The leakage angular fluxes are approximated by exponential forms, which allows to determine a closed-form solution for the photons transport equation. The angular flux and the parameters of the medium are used for the calculation of the absorbed energy in rectangular domains with different dimensions and compositions. In this study, only the absorbed energy by Compton effect is considered. We present numerical simulations and comparisons with results obtained by using the simulation platform GEANT4 (version 9.1) with its low energy libraries.

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## 1. Introduction

Modern procedures for physical-medical diagnosis and imaging is becoming increasingly sophisticated and thus need computer simulation approaches in order to investigate performance of methods and instruments. Radiation transport equations are the starting point to meet the challenges involved in developing and operating these instruments and methods. In order to be reliable, simulations shall adequately represent the physical processes involved. Many approaches for transport phenomena start from the Boltzmann equation, where one finds applications in transport problems from astrophysics to traffic flow (Badruzzaman, 1986). Elegant analytical and numerical techniques have been developed to solve the Boltzmann equation for a broad class of transport and radiative transfer problems. These methods follow two distinct schools of thought: the probabilistic school, such as the Monte Carlo methods that solve the exact problem approximately, and the deterministic school, such as the discrete ordinate methods, which give an exact (closed-form) solution for an approximate problem. Questions regarding accuracy and efficiency of deterministic transport methods are still an open issue even with modern super-computers. The most versatile and widely used deterministic methods are the  $P_N$  approximation (Davison, 1957; Segatto et al., 2000), the  $S_N$  approach (discrete ordinate method) (Vilhena and Barichello, 1995; Vilhena et al., 1995) and their variants (Segatto and Vilhena, 1994; Rodriguez, 2007). In discrete ordinate formulations of the transport equation, one assumes that the linearised Boltzmann equation holds only for a set of distinct numerical values of the direction-of-motion variables.

In the last decade, the  $LTS_N$  method was presented in the literature. This method solves, analytically, the discrete ordinates equation ( $S_N$  equation) in a slab by the Laplace transform technique. The main idea understands the following steps: application of the Laplace transform technique to the set of  $S_N$  equations, solution of the resulting algebraic equation by matrix diagonalization and last, inversion of the transformed angular flux by a standard procedure of Laplace transform theory. Here, analytical solution means that no approximation is made along the derivation of the solution, and its convergence is proven mathematically in Pazos and Vilhena (1999, 2000). This methodology has been applied for a broad class of transport and radiative transfer problems. In the further are given a few references, which the authors consider relevant for the present work: the LTS<sub>N</sub> solution for radiative transfer problem without azimuthal symmetry with severe anisotropy (Batistela et al., 1997) and an application of the  $LTS_N$  method on an inverse problem in hydrological optics (Velho et al., 2003). In

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a previous work (Rodriguez et al., 2006) the  $LTS_N$  method was applied in the solution of the one-dimensional transport equation with a Klein–Nishina scattering kernel and multi-group model for the wavelength variable. Numerical simulations showed that the resulting method generated solutions for transport problems in an heterogeneous slab that coincide with those from a GEANT4 Monte Carlo simulation (Wright, 2001; Agostinelli et al., 2003).

As an extension of the one dimensional approach we determine the solution of the two-dimensional transport equation considering the Klein–Nishina scattering kernel and a multi-group model. To this end the bi-dimensional  $LTS_N$  nodal approach is applied to a homogeneous and a heterogeneous rectangular domain. The main idea of the procedure discussed below relies on the solution of the two one-dimensional  $S_N$  equations resulting from transverse integration of the  $S_N$  equations in the rectangle by the  $LTS_N$  method, considering the leakage angular fluxes approximated by an exponential. Note, that the explicit form of the leakage angular flux is necessary in order to determine a closed-form solution for the transport equation, but the specific choice maid in this work does not restrict generality of the approach. A mathematical proof of convergence of the  $LTS_N$  nodal solution is discussed in Hauser et al. (2005).

In our numerical experiments we assume mono-energetic (E = 1.25 MeV) and mono-directional photon beam incident on the edge of a rectangle which is composed by water, bone or soft tissue, according the description of NCRP Report 44 (National Council of Radiation Protection and Measurements, 1975). We considered homogeneous as well as heterogeneous rectangular target media. The incoming photons are tracked until their whole energy is deposited or they leave the domain of interest. In this study only the Compton effect will be considered as interaction mechanism, which is justified by the fact that in the energy range of interest and for low Z the Compton effect is the dominant process for energy deposit, so that remaining effects may be neglected. Energy deposit is determined for a collection of spatial points of interest and compared to GEANT4 simulations (version 9.1) which makes use of low energy libraries for a two-dimensional problem. It is noteworthy, that previous versions of GEANT4 vielded different results, which indicates that developments of the Compton scattering package are still in progress.

Our article is organised as follows. In Section 2 we describe in detail  $LTS_N$  nodal solution of the Boltzmann transport equation in a rectangular domain assuming the Klein–Nishina scattering kernel and multi-group model. In Section 3 we report on numerical simulations for the absorbed energy in homogeneous and heterogeneous rectangular target media and compare our findings with results obtained from an implementation using the GEANT4 (version 9.1) platform (Wright, 2001). Finally, in Section 4 we present some concluding remarks and suggestions for future work.

#### 2. The LTS<sub>N</sub> nodal solution in a rectangular domain

The two-dimensional transport problem for the spectral angular flux  $I(x, y, \lambda, \Omega)$  contains besides a linear attenuation term (with coefficient  $\gamma_{ij}$ ) also a Klein–Nishina single scattering term. Here  $\lambda$ denotes the dimensionless wave length in multiples of the Compton wavelength. The integral over initial wavelengths (before scattering) may be decomposed into *G* intervals, where each of them corresponds to an energy group. A further modification of the continuous problem enters upon substitution of the Klein–Nishina differential cross section in the angular integral by a finite expansion in terms of Legendre polynomials  $P_{l}$ , a target matter parameter  $\alpha$ , which depends on the atom number, the atom mass number, the density of the target matter and the Thomson cross section, besides the Klein–Nishina scattering kernel  $k_{ri}$ . The angular integral may be replaced by an approximation using Gaussian quadrature with weights  $\omega_i$ . These modifications lead to the two-dimensional multi-group  $S_N$  nodal problem.

$$\begin{aligned} \mu_n \frac{\partial}{\partial x} I_{jn}(x, y) &+ \eta_n \frac{\partial}{\partial y} I_{jn}(x, y) + \gamma_{lj} I_{jn}(x, y) \\ &= \frac{\Delta}{3} \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{r=1}^{G} c_r \alpha k_{rj} P_l(1 + \lambda_r - \lambda_j) P_l(\mu_n) \sum_{i=1}^{N} P_l(\mu_i) I_{ri}(x, y) \omega_i, \end{aligned}$$

$$\tag{1}$$

subject to vacuum boundary conditions in a rectangular domain 0 < x < a and 0 < y < b. Here j = 1, ..., G is the energy group index, n = 1, ..., N, denotes the discrete angular directions, N = M(M + 2)/2 is the cardinality of the discrete ordinate set (number of discrete directions), M represents the order of the angular quadrature, the angular flux  $I_{jn}(x,y) = I(x,y, \lambda_j, \Omega_n)$  into the discrete direction  $\Omega_n = (\mu_n, \eta_n)$  for the *j*th group, the values of  $\omega_i$  are the Lewis and Miller quadrature weights (Lewis and Miller, 1984). In Eq. (1)  $\Delta$  signifies the interval from Simpson integration over the initial wavelengths, and  $c_r$  is a spectral weight. Further, the Klein–Nishina scattering kernel is known as

$$k_{rj} = k(\lambda_r, \lambda_j) = \frac{3}{8} \frac{\lambda_r}{\lambda_j} \left( \frac{\lambda_r}{\lambda_j} + \frac{\lambda_j}{\lambda_r} - \sin^2 \theta \right).$$
(2)

where  $\theta$  is the scattering angle and  $\lambda$  is the wavelength. In Rodriguez (2007) the one-dimensional problem was solved. Thus, the same procedure may be used without major changes once the spatial transverse variable is integrated out, which yields the set of two coupled  $S_N$  equations:

$$\eta_n \frac{\partial}{\partial y} I_{jny}(y) + \frac{\mu_n}{a} \left[ I_{jn}(a, y) - I_{jn}(0, y) \right] + \gamma_{lj} I_{jny}(y) = \frac{\Delta}{3} \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{r=1}^{G} c_r \alpha k_{rj} P_l(1 + \lambda_r - \lambda_j) P_l(\mu_n) \sum_{i=1}^{N} P_l(\mu_i) I_{riy}(y) \omega_i,$$
(3)

for all energy groups j = 1, ..., G, and all angular directions n = 1, ..., N. Here  $I_{jn}(a, y)$  and  $I_{jn}(0, y)$  are the angular fluxes that exit at the boundary and the average angular flux is  $I_{jny}(y) = \frac{1}{a} \int_{0}^{a} I_{jn}(x, y) dx$ . In analogy the integration over the longitudinal variable results in

$$\mu_n \frac{\partial}{\partial x} I_{jnx}(x) + \frac{\eta_n}{b} \left[ I_{jn}(x,0) - I_{jn}(x,b) \right] + \gamma_{lj} I_{jnx}(x)$$

$$= \frac{\Delta}{3} \sum_{l=0}^{L} \frac{2l+1}{2} \sum_{r=1}^{G} c_r \alpha k_{rj} P_l(1+\lambda_r-\lambda_j) P_l(\mu_n) \sum_{i=1}^{N} P_l(\mu_i) I_{rix}(x) \omega_i,$$
(4)

for j = 1, ..., G, n = 1, ..., N. Here  $I_{jn}(x, b)$  and  $I_{jn}(x, 0)$  is the angular flux that exits at the respective boundary. The average angular flux is  $I_{jnx}(x) = \frac{1}{b} \int_{0}^{b} I_{jn}(x, y) dy$ .

The previously introduced step prepared the system for application of the  $LTS_N$  method. Laplace transform renders the differential equation an inhomogeneous linear equation so that Eq. (4) reads now

$$s\overline{I_{jny}(s)} + \frac{\gamma_{lj}}{\eta_n}\overline{I_{jny}(s)} - \frac{\Delta}{3\eta_n}\sum_{l=0}^L \frac{2l+1}{2}\sum_{r=1}^G c_r \alpha k_{rj}P_l(1+\lambda_r-\lambda_j)P_l(\mu_n)$$
$$\times \sum_{i=1}^N P_l(\mu_i)\overline{I_{riy}(s)}\omega_i = I_{jny}(0) - \frac{\mu_n}{a\eta_n}\Big[\overline{I_{jn}(a,s)} - \overline{I_{jn}(0,s)}\Big], \tag{5}$$

for j = 1, ..., G and n = 1, ..., N.

The transformed solution for Eq. (4) is then given by

$$\overline{I_{jny}(s)} = (sI - B_{jny})^{-1} [I_{jny}(0) + \overline{Z_{(j-1)y}(s)} + \overline{S_{jny}(s)}].$$
(6)

Here  $\overline{I_{jny}(s)} = (\overline{I_{j1y}(s)}, \overline{I_{j2y}(s)}, \dots, \overline{I_{jNy}(s)})^T$  are the *N* components of the Laplace transformed angular flux vector in the *y* variable and  $I_{j-ny}(0) = (I_{j1y}(0), I_{j2y}(0), \dots, I_{jNy}(0))^T$  are the *N* components of the angular flux vector at *y* = 0. The components of matrix  $B_{jny}$  are given by

$$b_{y}(p,q) = \begin{cases} -\frac{\gamma_{ij}}{\eta_{p}} + \frac{\Delta}{3\eta_{p}} \sum_{l=0}^{L} \frac{2l+1}{2} c_{j} \alpha k_{jj} P_{l}(\mu_{p}) P_{l}(\mu_{p}) \omega_{q} & \text{if } p = q, \\ \frac{\Delta}{3\eta_{p}} \sum_{l=0}^{L} \frac{2l+1}{2} c_{j} \alpha k_{jj} P_{l}(\mu_{p}) P_{l}(\mu_{q}) \omega_{q} & \text{if } p \neq q, \end{cases}$$
(7)

and the scattering term reads

$$\overline{Z_{(j-1)y}(s)} = \sum_{i=1}^{j-1} H_{iy}\overline{I_{iny}(s)},$$
(8)

where the entries of the constant matrix  $H_{iy}$  are

$$h_{y}(p,q) = \begin{cases} \frac{\Lambda}{3\eta_{p}} \sum_{l=0}^{L} \frac{2l+1}{2} c_{i} \alpha k_{ij} P_{l}(1+\lambda_{i}-\lambda_{j}) P_{l}(\mu_{p}) P_{l}(\mu_{p}) \omega_{q} & \text{if } p = q, \\ -\frac{\Lambda}{3\eta_{p}} sum_{l=0}^{L} \frac{2l+1}{2} c_{i} \alpha k_{ij} P_{l}(1+\lambda_{i}-\lambda_{j}) P_{l}(\mu_{p}) P_{l}(\mu_{q}) \omega_{q} & \text{if } p \neq q, \end{cases}$$

$$(9)$$

The vector  $\overline{S_{jny}(s)}$  has the generic component

$$\overline{S_{jny}(s)} = -\frac{\mu_n}{a\eta_n} \Big[ \overline{I_{jn}(a,s)} - \overline{I_{jn}(0,s)} \Big].$$
(10)

An analogue procedure in the *x* variable leads to the  $LTS_N$  nodal solution for Eq. (5)

$$\overline{I_{jnx}(s)} = (sI - A_{jnx})^{-1} [I_{jnx}(0) + \overline{Z_{(j-1)x}(s)} + \overline{S_{jnx}(s)}].$$
(11)

Here  $\overline{I_{j_{IIX}}(s)} = (\overline{I_{j_{1X}}(s)}, \overline{I_{j_{2X}}(s)}, \dots, \overline{I_{j_{NX}}(s)})^T$  are the *N* components of the Laplace transformed angular flux vector in the *x* variable and  $I_{j_{II-x}}(0) = (I_{j_{1X}}(0), I_{j_{2X}}(0), \dots, I_{j_{NX}}(0))^T$  are the *N* components of the angular flux vector at *x* = 0. The entries of matrix  $A_{j_{NX}}$  are

$$a_{x}(p,q) = \begin{cases} -\frac{\gamma_{ij}}{\mu_{p}} + \frac{\Lambda}{3\eta_{p}} \sum_{l=0}^{L} \frac{2l+1}{2} c_{j} \alpha k_{jj} P_{l}(\mu_{p}) P_{l}(\mu_{p}) \omega_{q} & \text{if } p = q, \\ \\ \frac{\Lambda}{3\mu_{p}} \sum_{l=0}^{L} \frac{2l+1}{2} c_{j} \alpha k_{jj} P_{l}(\mu_{p}) P_{l}(\mu_{q}) \omega_{q} & \text{if } p \neq q, \end{cases}$$
(12)

and the scattering term reads

$$\overline{Z_{(j-1)x}(s)} = \sum_{i=1}^{j-1} H_{ix}\overline{I_{inx}(s)},$$
(13)

where the constant matrix  $H_{ix}$  has the elements

$$h_{x}(p,q) = \begin{cases} \frac{\Lambda}{3\mu_{p}} \sum_{l=0}^{L} \frac{2l+1}{2} c_{i} \alpha k_{ij} P_{l}(1+\lambda_{i}-\lambda_{j}) P_{l}(\mu_{p}) P_{l}(\mu_{p}) \omega_{q} & \text{if } p = q, \\ -\frac{\Lambda}{3\mu_{p}} \sum_{l=0}^{L} \frac{2l+1}{2} c_{i} \alpha k_{ij} P_{l}(1+\lambda_{i}-\lambda_{j}) P_{l}(\mu_{p}) P_{l}(\mu_{q}) \omega_{q} & \text{if } p \neq q, \end{cases}$$
(14)

and the vector  $\overline{S_{jnx}(s)}$  is

$$\overline{S_{jnx}(s)} = -\frac{\eta_n}{b\mu_n} \Big[ \overline{I_{jn}(s,b)} - \overline{I_{jn}(s,0)} \Big].$$
(15)

In order to determine the angular fluxes the inverse Laplace transform is applied to Eqs. (6) and (11).

$$I_{jny}(y) = \mathcal{L}^{-1}\{(sI - B_{jny})^{-1}[I_{jny}(0) + \overline{Z_{(j-1)y}(s)} + \overline{S_{jny}(s)}]\},$$
(16)

$$I_{jnx}(x) = \mathcal{L}^{-1}\{(sI - A_{jnx})^{-1}[I_{jnx}(0) + \overline{Z}_{(j-1)x}(s) + \overline{S}_{jnx}(s)]\},$$
(17)

One of the standard inversion methods is given by the Heaviside expansion

$$\begin{split} I_{jny}(y) &= \sum_{k=1}^{jn} \beta_k e^{s_k y} I_{jny}(0) + Z_{(j-1)y}(y) * \mathcal{L}^{-1} \{ (sI - B_{jny})^{-1} \} \\ &+ S_{jny}(y) * \mathcal{L}^{-1} \{ (sI - B_{jny})^{-1} \}, \end{split}$$
(18)

and

$$\begin{split} I_{jnx}(x) &= \sum_{k=1}^{jn} \beta_k e^{s_k x} I_{jnx}(\mathbf{0}) + Z_{(j-1)x}(x) * \mathcal{L}^{-1}\{(sI - A_{jnx})^{-1}\} \\ &+ S_{jnx}(x) * \mathcal{L}^{-1}\{(sI - A_{jnx})^{-1}\}. \end{split}$$
(19)

Here the star operator denotes convolution.

To complete the solution still depends on the unknown leakage angular fluxes at the boundary, namely  $I_{jn}(x, 0)$ ,  $I_{jn}(0, y)$ ,  $I_{jn}(x, b)$  and  $I_{jn}(a, y)$ . To this end we follow the work of Hauser et al. (2002) which states that the exponential approximation gives the best results for the two-dimensional  $LTS_N$  nodal solution for deep penetration problems. Note, that for the procedure discussed here there are no restrictions on the specific form of the leakage angular flux except that it shall be analytical in order to obtain an analytical expression for the solution of the problem.

$$\begin{split} I_{jn}(x,0) &= F_{jn} e^{-\operatorname{sign}(\mu_n)Ax},\\ I_{jn}(0,y) &= G_{jn} e^{-\operatorname{sign}(\eta_n)Ay},\\ I_{jn}(x,b) &= O_{jn} e^{-\operatorname{sign}(\mu_n)Ax},\\ I_{jn}(a,y) &= P_{jn} e^{-\operatorname{sign}(\eta_n)Ay}, \end{split}$$
(20)

where  $sign(\mu)$  denotes the signal function:

$$sign(\mu) = \begin{cases} 1 & \text{if } \mu > 0, \\ -1 & \text{if } \mu < 0, \end{cases}$$
(21)

and  $\Lambda$  represents the decay constant parameter, which has to be chosen a priori. In this work, we assume  $\Lambda$  (see also Hauser et al., 2002) to represent the absorption cross section

$$\Lambda = \sigma_a = \sigma_t - \sigma_s. \tag{22}$$

The functions  $sign(\mu_n)$  and  $sign(\eta_n)$  which appear in Eq. (20) guarantee that the approximated angular fluxes will decay for any discrete direction. Replacing (20) in Eqs. (18) and (19) then the *x*-averaged and *y*-averaged angular fluxes solutions are complete after the Laplace Transform inversion. Applying the boundary conditions determines the integration constants so that the two-dimensional *LTS<sub>N</sub>* nodal solution is well determined. The *LTS<sub>N</sub>* nodal solution may be generalised for a heterogeneous rectangular medium, applying the *LTS<sub>N</sub>* solution for a homogeneous medium to each sub-domain and evaluate the integration constants applying boundary and interface conditions.

## 3. Numerical results

The solution derived in the previous section is applied to different cases, where geometry and matter composition vary (water, soft tissue or bone). We report on the numerical simulations for the absorbed energy in the rectangular domains for the six case studies, specified in more detail below. As projectile a mono-energetic and mono-directional photon beam (E = 1.25 MeV) is considered, incoming on the edge of a rectangle. The incoming photons will be tracked until their whole energy is deposited or they leave the domain of interest. Because of the fact that for the initial photon energy and for the afore mentioned target matter composition the Compton effect dominates, one expects by comparison to GEANT4 simulations that other physical processes will have only spurious effects and may be neglected.

The data were simulated using the GEANT4 platform (Allison et al., 2006; Kelley et al., 1972) (version 9.1), which is a well estab-

lished tool-kit for simulating the passage of particles through matter. It includes a complete range of functionality including tracking, geometry, physics models and hits. The list of interactions covers besides electromagnetic also hadronic and optical processes. The simulator recognizes a large set of long-lived particles, materials and elements, with interaction data over a wide energy range, starting in some cases from 250 eV and extending in others up to TeV. The program platform has been designed and constructed to expose the physics models utilized, to handle complex geometries and to enable its easy adaptation for optimal use in different sets of applications.

The computational universe considered in this work contains a mono-energetic and unidirectional photon source aligned with the y-axis and incident in the centre line of the sheet. The geometries have been chosen in a way to prevent particle loss on the lateral borders. Table 1 shows the considered geometries, where the sensitive volume is understood as the volume of a specific material where energy is deposited. For each simulation 10<sup>6</sup> histories were generated. The G4EMLowEnergy low energy library is based on the Livermore Library. The cut-off energies applied for sensitive volume of water are 1.09571 keV for photons and 84.2696 keV for electrons, considering the bone cortical and soft tissue they are 1.10688 keV for photons and 86.3701 keV for electrons. These cut-off energies signify that particles or photons with energies lower than this threshold deposit their remaining energy in this step. From the GEANT4 physics process list we activated the photoelectric effect, Compton scattering, Rayleigh scattering, and the low energy electron processes.

In the following the six case studies, each for a variety of geometries, are presented.

*Case 1:* The first case considers an incoming photon beam aligned with the *y* axis and incident on three sheet geometries (20 cm  $\times$  10 cm, 20 cm  $\times$  20 cm and 30 cm  $\times$  40 cm) for a homogeneous target of water with charge to mass ratio *Z*/*A* = 0.55508 and density  $\rho$  = 1 g/cm<sup>3</sup>. Further vacuum boundary conditions are understood. The results represent the average absorbed energy in units of keV per incoming photon and are shown in Table 2 for the *LTS<sub>N</sub>* solution and the GEANT4 simulations.

#### Table 1

Target sheet geometry for the homogeneous and non-homogeneous cases. In the homogeneous cases the materials water, bone and soft tissue fill entirely each rectangle. In the non-homogeneous cases the depth of the entrance medium  $(v_1)$  is 1 cm or 5 cm and the remaining depth is filled with the second medium  $(v_2)$ . The material combinations are water-bone and bone-water.

	Dimensions	
	<i>x</i> (cm)	<i>y</i> (cm)
Homogeneous sensitive volume	20 20 30	10 20 40
Non-homogeneous sensitive volume $v_1 \cup v_2$	20 20 30	10 20 40

#### Table 2

Absorbed energy in keV per photon incident on a homogeneous rectangular sheet composed by water liquid.

Domain dimension	LTS <sub>8</sub>	GEANT4	Discrepancy (%)
20 cm × 10 cm 20 cm × 20 cm	0.00309 0.00457	0.00315 0.00468	1.9 2.3
$30 \text{ cm} \times 40 \text{ cm}$	0.01140	0.01160	1.7

- *Case 2:* To check the influence of the material density in the absorbed energy calculation, let us consider a rectangular domain composed by bone cortical (*Z*/*A* = 0.51478,  $\rho$  = 1.92 g/cm<sup>3</sup>) and vacuum boundary conditions.
- *Case 3:* This case considers a homogeneous rectangular sheet composed by soft tissue with Z/A = 0.54996 and  $\rho = 1.06 \text{ g/cm}^3$  and vacuum boundary conditions.

For the three case studies the numerical results for the energy deposit of the  $LTS_N$  method together with the GEANT simulations are shown in Tables 2–4. Although the  $LTS_N$  considered only the Compton contribution whereas the GEANT simulation included other interactions the maximum discrepancy found was lower than 4%, which in turn justifies the validity of the present approach especially by virtue of having used two different methods.

- *Case 4:* Biological targets subject to radiation treatment have often a multi-layer structure. The simplest model in this direction considers two layers, the first one of 1 cm depth filled with water liquid (Z/A = 0.55508,  $\rho = 1$  g/ cm<sup>3</sup>) and the second one (with depths of 9 cm, 19 cm and 39 cm, resp.) composed by bone cortical (Z/A = 0.51478,  $\rho = 1.92$  g/cm<sup>3</sup>). Further vacuum boundary conditions are understood.
- *Case 5:* In order to get an idea on the influence of the thickness of the first layer on the energy deposit in the heterogeneous rectangular sheet containing water and bone, the thickness of the entrance sheet (containing water) of the previous case was changed to 5 cm while the matter specification, the dimension of the total and boundary conditions remained the same.
- *Case 6:* A further comparison to case 4 was performed interchanging the materials for the entrance and subsequent layer. The surface layer of 1 cm depth contained bone cortical (*Z*/*A* = 0.51478,  $\rho$  = 1.92 g/cm<sup>3</sup>) and the second layer was composed by water liquid (*Z*/*A* = 0.55508,  $\rho$  = 1 g/cm<sup>3</sup>) and additionally vacuum boundary conditions.

In Table 6 we report on the *LTS*<sub>8</sub> numerical results together with the GEANT simulation findings for the absorbed energy in a heterogeneous rectangular geometry composed by water liquid and bone cortical with an entrance layer of 5 cm depth. In Tables 5 and 7 the *LTS*<sub>8</sub> and GEANT simulations are shown for the absorbed energy in a double layer rectangular sheet composed either of water liquid and bone cortical or with both materials interchanged. The depth of the entrance layer was 1 cm. As already observed in

Table 3

Absorbed energy in keV per photon incident on a homogeneous rectangular sheet composed by bone cortical (ICRU, 1989).

Domain dimension	LTS <sub>8</sub>	GEANT4	Discrepancy (%)
$\begin{array}{c} 20\ \text{cm}\times10\ \text{cm}\\ 20\ \text{cm}\times20\ \text{cm}\\ 30\ \text{cm}\times40\ \text{cm} \end{array}$	0.05588	0.05781	3.3
	0.09087	0.09405	3.4
	0.15771	0.16375	3.7

## Table 4

Absorbed energy in keV per photon incident on a homogeneous rectangular sheet composed by soft tissue (ICRU, 1989).

Domain dimension	LTS <sub>8</sub>	GEANT4	Discrepancy (%)
20 cm × 10 cm	0.00307	0.00313	1.9
20 cm × 20 cm	0.00531	0.00542	2.0
30 cm × 40 cm	0.01523	0.01560	2.4

#### Table 5

Absorbed energy in keV per photon incident on a heterogeneous rectangular sheet composed by water liquid with 1 cm depth ( $v_1$ ) followed by bone cortical of 9 cm, 19 cm or 39 cm depth ( $v_2$ ), resp. (ICRU, 1989).

Domain dimension $v_1 \cup v_2$	Sensitive volume	LTS <sub>8</sub>	GEANT4	Discrepancy (%)
$20 \text{ cm} \times 10 \text{ cm}$	$v_1$	0.00015	0.00016	6.2
	$v_2$	0.05289	0.05549	4.5
$20 \text{ cm} \times 20 \text{ cm}$	$v_1 \\ v_2$	0.00017 0.08629	0.00018 0.09089	5.6 5.1
$30\ cm\times 40\ cm$	$v_1$	0.00018	0.00019	5.3
	$v_2$	0.15322	0.16098	4.8

#### Table 6

Absorbed energy in keV per photon incident on a heterogeneous rectangular sheet composed by water liquid with 5 cm depth ( $v_1$ ) followed by bone cortical of 5 cm, 15 cm or 35 cm depth ( $v_2$ ), resp. (ICRU, 1989).

Domain dimension $v_1 \cup v_2$	Sensitive volume	LTS <sub>8</sub>	GEANT4	Discrepancy (%)
$20 \text{ cm} \times 10 \text{ cm}$	$v_1$	0.00091	0.00095	4.2
	$v_2$	0.13476	0.14375	4.4
$20\ cm \times 20\ cm$	$v_1 \\ v_2$	0.00113 0.06909	0.00117 0.07221	3.4 4.3
$30 \text{ cm} \times 40 \text{ cm}$	$v_1$	0.00131	0.00137	4.4
	$v_2$	0.13765	0.14376	4.2

#### Table 7

Absorbed energy in keV per photon incident on a heterogeneous rectangular sheet composed by bone cortical with 1 cm depth ( $v_1$ ) followed by water liquid of 9 cm, 19 cm or 39 cm depth ( $v_2$ ), resp. (ICRU, 1989).

Domain dimension $v_1 \cup v_2$	Sensitive volume	LTS <sub>8</sub>	GEANT4	Discrepancy (%)
$20 \text{ cm} \times 10 \text{ cm}$	$v_1$	0.00225	0.00243	7.4
	$v_2$	0.00277	0.00296	6.4
$20 \text{ cm} \times 20 \text{ cm}$	$v_1 \\ v_2$	0.00403 0.00425	0.00427 0.00451	5.6 5.8
$30 \text{ cm} \times 40 \text{ cm}$	$v_1$	0.00711	0.00758	6.2
	$v_2$	0.01068	0.01142	6.5

the homogeneous study cases also in the heterogeneous calculations the discrepancies were found to be lower than 8%.

From the analysis of the results encountered for the six cases one can confirm a good agreement between the proposed methodology and the results by the Monte Carlo technique. All calculations were performed on microcomputers; the  $LTS_N$  nodal calculations were implemented on an AMD Athlon 1700 (1.4 GHz) computer while the Geant4 results are obtained using a Pentium 4 (1.7 GHz) hardware. The maximum computational time necessary to generate the results for each case did not exceed 30 min for both methods, the  $LTS_N$  nodal approach and the Monte Carlo simulation by the GEANT platform.

### 4. Conclusions

The present work focussed on the derivation of a closed-form solution for a two-dimensional transport equation that considers photons incident on a rectangular sheet which contained a mono-or double-layer with specific material specification. The  $S_N$  transport equation was solved for energy deposit in the material using the  $LTS_N$  nodal approach. Since the mathematical proof of convergence of this type of approach classifies the closed-form solution an almost exact solution in the sense that once a precision

of the solution is required one may determine the number of discrete directions and the number of wavelength groups that comply with the specification.

The energy of the photon beam in the range below and up to *MeV* energies indicates the Compton effect as the dominant process for photon (biological) matter interaction, thus the Klein–Nishina scattering kernel was implemented in a multi-group model. The comparison with GEANT4 simulations, which is based on a physical Monte Carlo simulation, showed that for the considered energy the Compton scattering kernel is sufficient to reproduce the energy deposit with less than 5–10% discrepancy. It is noteworthy, that the GEANT results are systematically but only slightly higher than the *LTS<sub>N</sub>* calculations, which is to be expected since the used process list in the Monte Carlo simulations contains other processes besides the Compton effect.

In order to uniquely determine the solution an assumption for the leakage angular flux was necessary, which was approximated by exponential forms. Although the form seems to lack generality, nevertheless, for the present considerations the specific approximation was the result of a variety of trials where the adopted form suited best in order to reproduce results from other approaches. Details of this analysis may be found in Hauser et al. (2002). Moreover, the explicit form of the leakage angular flux is necessary in order to determine a closed-form solution for the transport equation, but the specific choice maid in this work does not restrict the generality of the approach, other forms are possible and may be used to fix ambiguities of the solution.

The agreement that was found between the GEANT results and the present approach permit to use the  $LTS_N$  solution as input for Monte Carlo simulations. Longer term practice with GEANT4 showed that, although its flexibility with respect to complexity of geometries and materials used in specific problems that may be simulated, computational time increases almost exponentially the larger the layer structure becomes. The  $LTS_N$  approach has a polynomial increase in computational time, so that the energy deposit in small patches of a multi-layer structure may be simulated using the results from such a solution. Evidently, the important question of the specific form of leakage angular fluxes has to be solved, which we postpone to a future work. As a next step we focus our future attention to the extension of the present approach for the solution of the three-dimensional transport problem in Cartesian geometry.

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