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MONTE CARLO SIMULATION FOR RADIATION TRANSPORT: COLLISION DENSITY IN A 1-D SLAB

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ABSTRACT
Monte Carlo (MC) simulation has been abundantly used for simulation of radiation transport (thermal, neutron, charged-particle etc) in matter. In thermal radiation, for example, surface radiosities and subsequent heat fluxes have been accurately determined in configurations which are difficult for deterministic formulations. In this paper, we consider estimation of the collision density in a 1-D slab and compare with the exact solution. The accuracy of the simulation results is discussed and a Poisson distribution is shown for the events in a random walk. The purpose of this paper is to demonstrate the underlying simulation process for a simple problem.

Keywords: radiation transport, neutron transport, Monte Carlo simulation, collision density.

INTRODUCTION
Monte Carlo (MC) simulation has been abundantly used (see *e.g.* Spanier and Gelbard [1], Lamarsh [2], Brewster [3], Modest [4]) for simulation of radiation transport (thermal, neutron, charged-particle etc) in matter. In thermal radiation, problems of interest include high-temperature environments in boilers and furnaces, and irregular-geometry enclosures containing participative media such as combustive gases. Surface radiosities and subsequent heat fluxes have been accurately determined in configurations which are difficult for deterministic formulations. The attractiveness of MC schemes becomes more prominent in mixed-mode and coupled thermo-fluid problems, where the non-linearity, spectral characteristics and geometrical complexity may render deterministic treatments largely ineffective.

In this paper, we consider estimation of the collision density in a 1-D slab and the transmission probability. The thermal radiative transfer formulation is very similar to the neutron and photon transport as it based on the integral form of the Boltzmann equation. Traditionally, MC simulation is seen to be analogous to the Neumann series solution of the governing integral equation. Thus, we consider an idealized, extensively studied, 1-D slab transmission problem for which the exact solution is available.

MONTE CARLO SIMULATION
Monte Carlo (MC) simulation of radiation consists of sampling source particles, from a point or an emitting surface, and transporting them to their final destination using laws of probability. A simulation of N histories involves the following steps for a history

i. Selection of a source emissive power.
ii. Selection of emission angles θ and φ, as shown in Figure-1.
iii. Ray tracing in the direction of propagation.
iv. Determination of point of intersection, if any with the destination surface (Figure-2).
v. Determination of fate of history at the destination surface.

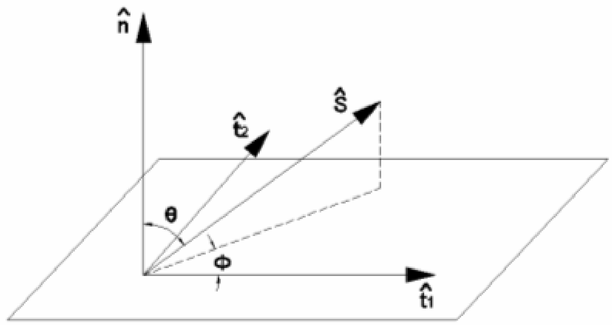

Figure-1. The vector of propagation $\hat{S}$ is related to the unit vectors $\hat{t}_1, \hat{t}_2$ *and* $\hat{n}$.

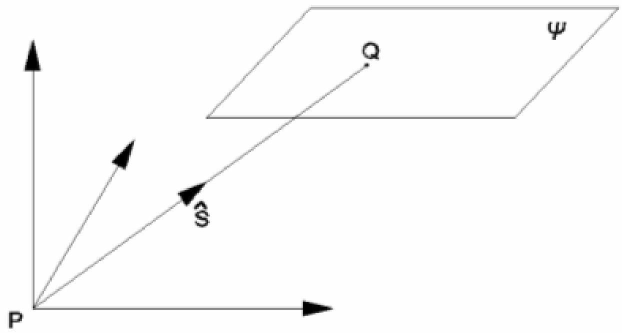

Figure-2. The point of intersection Q in the direction $\hat{s}$.

In case of thermal radiation, the sample size is determined from the emitted energy of a surface, $E = A\varepsilon e_b \equiv A\varepsilon\sigma T^4$. The procedure is to select N bundles, each bundle having energy ω such that $E = \omega N$, and to transport it to the destination surface. The point of emission P from a 2-D surface of length L and width W can be determined, in case of uniform emission, from $x_e = \xi_1 L, y_e = \xi_2 W$ where ξ is

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a uniformly distributed random number in the range (0, 1). The polar and azimuthal angles θ and φ respectively are determined as $\theta = \sin^{-1}(\sqrt{\xi_3})$ for a diffuse surface emitter, and $\phi = 2\pi\xi_4$. On intersection at *Q*, a scattering is chosen with probability $1-\varepsilon$ and thus $0 < \xi_5 \leq 1-\varepsilon$ determines a scattering whereas $1-\varepsilon < \xi_5 \leq 1$ corresponds to an absorption. In case of scattering, new angles (θ, φ) are determined and the process continues until the history is terminated on absorption. The quantity of interest in the problem is that energy exchange or equivalently, the difference between the energy emitted from a surface and absorbed by that surface.

The distance to collision s, is obtained from the PDF: $f(s)ds = K_t e^{-K_t s} ds$, from which, using a uniformly random number in the range (0,1) for the CDF, a distance to collision DTC, can be sampled as $s = -\frac{1}{K_t}\ln(1-\xi)$. The average value of the DTC, or the mean free path $<s>$ is then $<s> = \int_0^\infty s f(s) ds = \frac{1}{K_t}$. Alternately, in units of optical distance, also called the optical depth, $t = K_t s$, the mean optical path is then $<t> = 1$. Here, the absorption, scattering and total cross-sections are K_a, K_s and $K_t = K_a + K_s\ cm^{-1}$ and the optical thickness is $t = K_t z$.

The object of an MC simulation is to obtain an estimate that is both accurate and precise in the statistical sense *i.e.* a 'good' mean value and a 'small' variance.

COLLISION DENSITY IN A 1-D SLAB

We consider a unit beam source impinging on the left surface of a 1-D slab of optical thickness *T*. For simplicity, it is assumed that forward scattering takes place in the medium and collisions do not result in energy loss. This is one of the simplest cases for which results from the simulation can be compared with the exact analytical solution. The quantities of interest are the spatial collision density, $\psi(t)$ which is defined as the number of collisions per unit volume, and the transmission probability $J(T)$. For estimating the collision density, two estimators are used *viz* the collision estimator (CE), and the track-length estimator (TLE).

The simulation process in a slab of six regions is illustrated in Figure-3. A typical history begins with a weight *w=1*. A distance to collision is sampled, as described above, and the region is determined. The type of collision, *e.g.* absorption or scattering, is determined using random numbers, and in analog simulation the history is terminated when a particle is absorbed or escapes from the system.

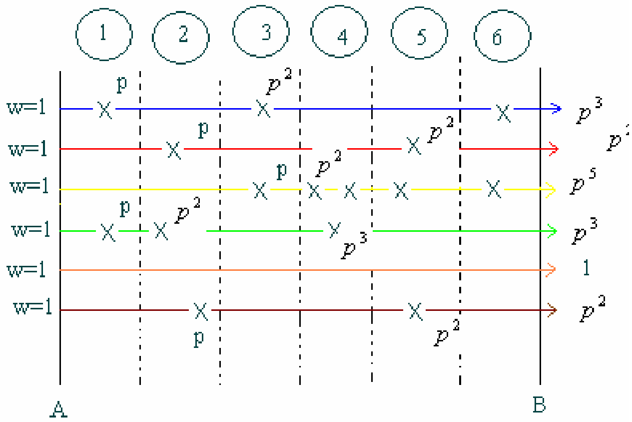

Figure-3. Forward scattering of incident photons in a 1-D slab with 6 regions.

Here, we use non-analog simulation where, for computational efficiency, the statistical weight of a particle is reduced to $p \equiv K_s / K_t$, the scattering probability. Consider the histories shown in Figure-1. The first history has three events of which the first collision is in region 1, the second collision in region 3 and the third collision in region 6. The weight of the particle emerging is $w = p^3$. Similarly, histories 2-5 are as shown in the Figure. The collision density $\psi(z)$, using a collision estimator, is then simply the 'weight' of the particles deposited in each region. Thus $\psi(z) = \sum_{n=0}^{\infty} p^n P(n \mid z)$ and the transmission probability is $J(T) = \psi(z = T)$. For a sample size of six particles, the collision density is $\psi_1 = p/3, \psi_2 = (2p + p^2)/6$ and so on. Similarly, the transmission probability is $J(T) = (p^3 + p^2 + p^5 + p^3 + 1 + p^2)/6$.

Mathematically, the above process can be modeled by an integral equation such as the Volterra equation of the second type which, for example, for the intensity of radiation $I(t, \mu)$ is

$$I(t,\mu) = I(0,\mu)\exp(-t/\mu) + \int_0^t I_b(t')\exp(\frac{t'-t}{\mu})\frac{dt'}{\mu}$$

For the case of forward scattering considered here, the cosine of the angle of scattering $\mu = \cos\theta$ is represented by $\delta(\mu - 1)$ and, the model reduces to

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$$I(t) = I(0)\exp(-t) + \int_0^t I_b(t^{'})\exp(t^{'}-t)dt^{'} \equiv S(t) + \int_0^t I(t^{'})p_s \exp(t^{'}-t)dt^{'}$$

This integral equation can be solved by the Neumann series method as follows:

assume initially that $I(t) \equiv I_0(t) \cong S(t) = e^{-t}$, use this in the integral equation to get

$$I_1(t) = S(t) + e^{-t}\int_0^t dt_1 \equiv e^{-t} + \int_0^t S(t_1)K(t_1 \to t)dt_1$$

and use $I_1(t)$ to get a 'better' solution

$$I_2(t) = S(t) + e^{-t}\int_0^t dt_1 \int_0^{t_1} dt_2 \equiv e^{-t} + \int_0^t \int_0^{t_1} dt_1 dt_2 S(t_1)K(t_1 \to t_2)K(t_2 \to t)$$

and so on. The Neumann series analytical solution to the above can then be written as $I(t) = I(0)e^{-t} + \sum_{n=1}^{\infty} I_n(t)$ where $I_n(t) = \int_0^t \int_0^{t_1} \Lambda \int_0^{t_{n-1}} dt_1 dt_2 \Lambda\, dt_n K(t_n \to t)\prod_{i=1}^{n-1} K(t_i \to t_{i+1})$.

In the above, the transition kernel $K(t_i \to t_{i+1})$ can be written as a 'collision' term $C_i = p_{s,i}$, the scattering probability at the i^{th} collision, and a 'transport' term $T(t_i \to t_{i+1}) = e^{-(t_{i+1}-t_i)}$ which transports the particle to the $(i+1)^{th}$ collision site. Thus the transition kernel is $K(t_i \to t_{i+1}) = C_i \cdot T_i$ where it is understood that C_i carries the pre-collision statistical 'weight' and properties of the particle, and T_i carries the post-collision information. This formulation, as will be shown in subsequent work, makes a perturbation analysis straight-forward. We can also attempt to write down a formulation for the stochastic process in which the random walk is treated in an analog manner with the only exception of allowing a particle to continue its 'history', or life, with a reduced 'weight' (equal to the pre-collision survival probability) even though it may actually have been absorbed. The complete set of events for a collision density or a transmission problem, whose probabilities must add up to unity, is then the contribution from events with zero collisions, with one collision, with two collisions and so on. When these are written, we will at once see the significance of the Neumann series solution which proceeded on purely mathematical grounds. The probabilities can be written as:

$$P_T(0 \mid T) = e^{-T}$$

$$P_T(1 \mid T) = \int_0^t dy_1 e^{-y_1} \cdot e^{-(T-y_1)} = e^{-T}\int_0^T dy_1 = e^{-T}T$$

$$P_T(2 \mid T) = \int_0^T dy_1 e^{-y_1} \cdot \int_{y_1}^T dy_2 \cdot e^{-(T-y_2)} = e^{-T}\int_0^T dy_1 \int_{y_1}^T dy_2 = e^{-T}\frac{T^2}{2!}$$

$$P_T(3 \mid T) = \int_0^T dy_1 e^{-y_1} \cdot \int_{y_1}^T dy_2 \cdot e^{-(y_2-y_2)} \int_{y_2}^T dy_3 \cdot e^{-(T-y_3)} = e^{-T}\int_0^T dy_1 \int_{y_1}^T dy_2 \int_{y_2}^T dy_3 = e^{-T}\frac{T^3}{3!}$$

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$$P_T(n \mid T) = \int_0^T dy_1 e^{-y_1} \cdot \int_{y_1}^T dy_2 \cdot e^{-(y_2-y_2)} \Lambda \int_{y_2}^T dy_n \cdot e^{-(T-y_n)} = e^{-T}\int_0^T dy_1 \int_{y_1}^T dy_2 \Lambda \int_{y_n}^T dy_n = e^{-T}\frac{T^n}{n!}$$

We have shown above that a Poisson distribution is obtained for the probability of each event, which needs to compared with the PDF obtained in a simulation. The exact solution for the collision density and the transmission probability can then be found as $\psi(t) = \sum_{n=0}^{\infty} p^n e^{-t}\frac{t^n}{n!} = e^{-(K_a/K_t)t}$ and $J((T) = e^{-(K_a/K_t)T}$ respectively. To test the accuracy of this estimate, we carry out simulations in the following stages:

i- carry out a simulation to estimate $<\psi>, \sigma_{<\psi>}$ and $<J(T)>, \sigma_{<J>}$

ii- compare above with exact results

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iii- construct a PDF, $< P(n \mid Z_o) >$ and compare with a Poisson PDF

A MATLAB® program was written for simulation, construction of a PDF from the simulation for the transmission through the last surface, and for comparison with the exact analytical solution for the collision density obtained from the integral equation. Figure-4 shows a simulation for a slab of $t = 10$ (optical thickness) with 20 regions, *i.e.* 0.5 optical thickness each. Since $< t >= 1$, the probability of having a collision in a region is small and the CE is bound to give an inaccurate result. This discrepancy, between the MC estimate and the exact result, remains (Figure-5) even as the sample size is increased to 100000X5. However, the results improve (Figure-6) as the size of the regions is increased from 0.5 to 1.0 optical units. Clearly, this is due to the fact that for the CE to provide reliable results in an MC simulation, the size of the region, or mesh in a deterministic analogy, must be larger than an optical unit. In case the mesh size can not be increased, the track-length estimator (TLE) should be used instead of the CE. Figure-7 shows the results for both MC simulation and exact solution for a slab thickness of 20 optical units.

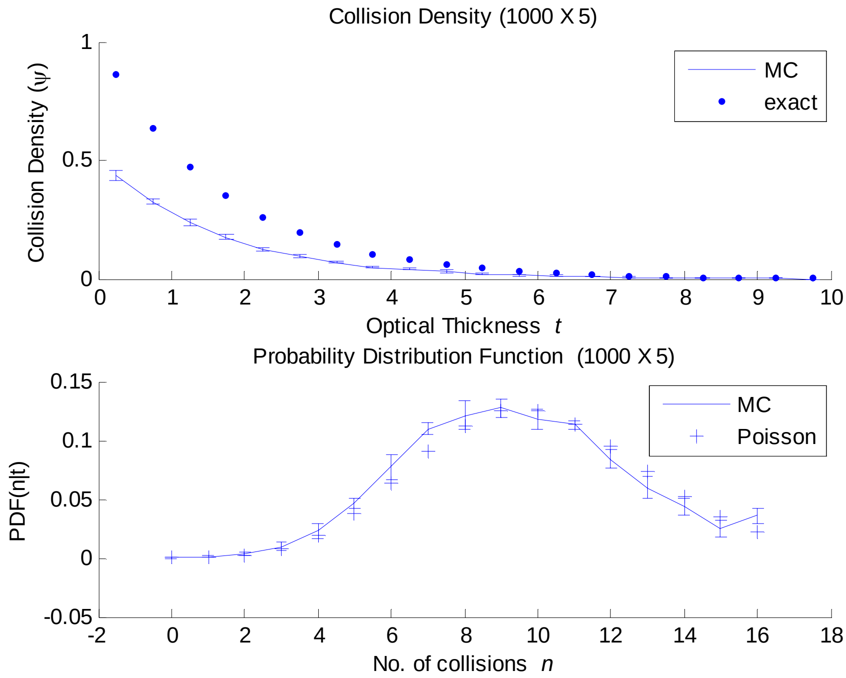

Figure-4. Monte Carlo simulation, 1000 particles and 5 batches, for a 1-D slab of thickness 10 optical units, with forward scattering and 20 regions.

Figures 4 and 7 also show the PDF of the number of collisions *n* given the slab thickness *t*. The estimated PDF is compared with the Poisson values for each slab. Finally Figure-8 shows the Poisson PDF for given slab thickness. These comparisons serve to get an intuitive understanding of the simulation process.

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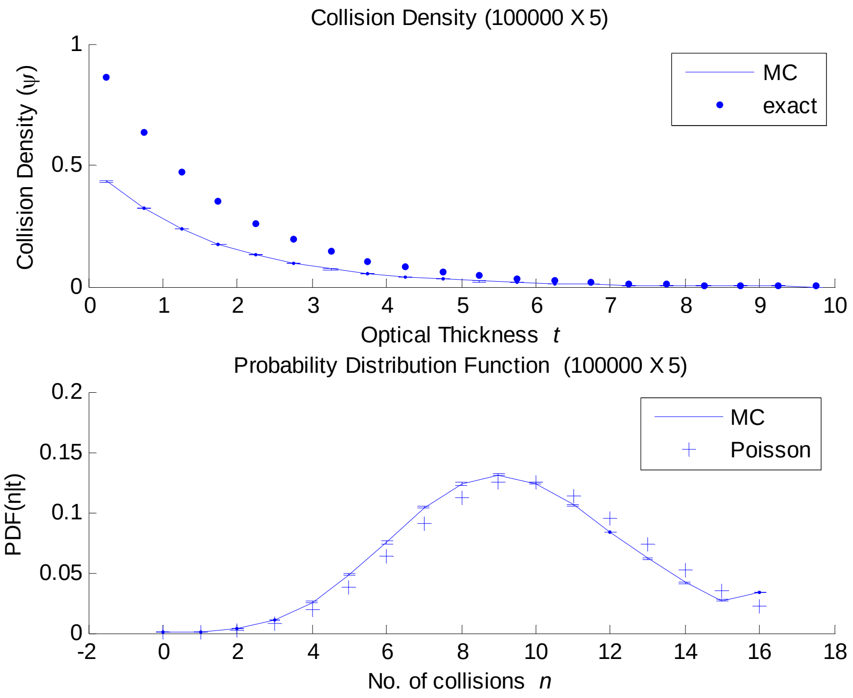

Figure-5. Monte Carlo simulation, 100000 particles and 5 batches, for a 1-D slab of thickness 10 optical units, with forward scattering and 20 regions.

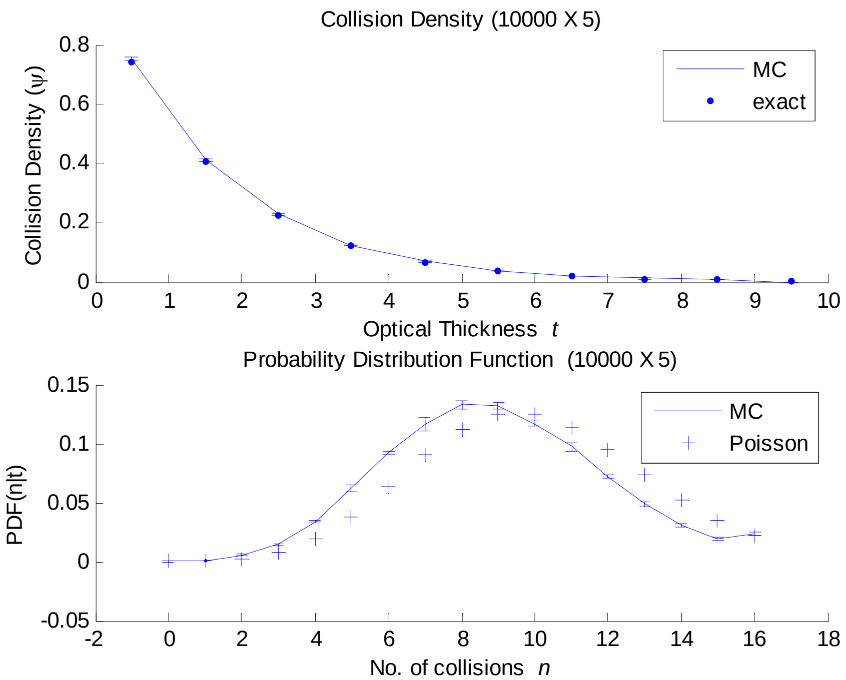

Figure-6. Monte Carlo simulation, 10000 particles and 5 batches, for a 1-D slab of thickness 10 optical units, with forward scattering and 10 regions.

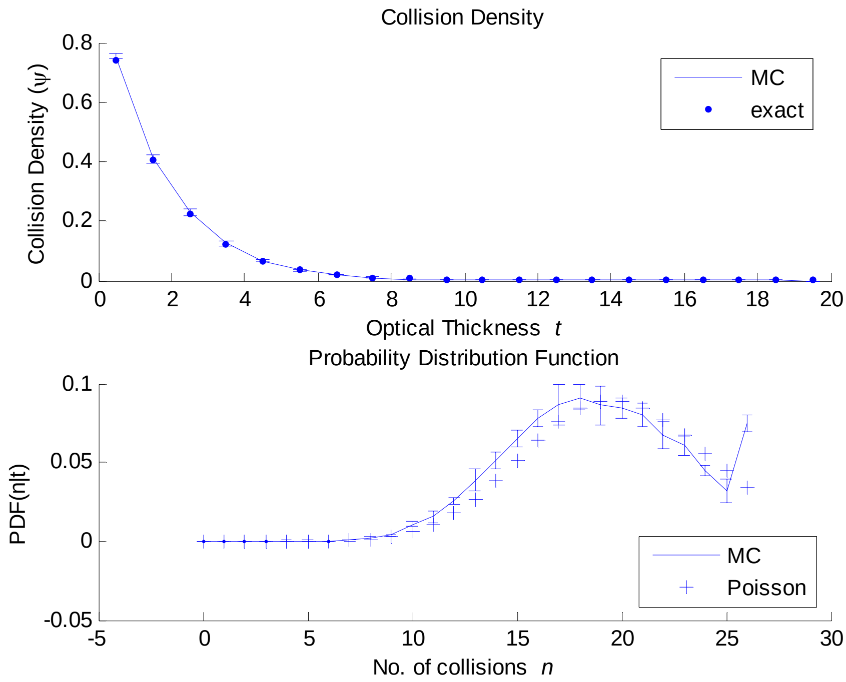

Figure-7. Monte Carlo simulation, 10000 particles and 5 batches, for a 1-D slab of thickness 20 optical units, with forward scattering and 20 regions.

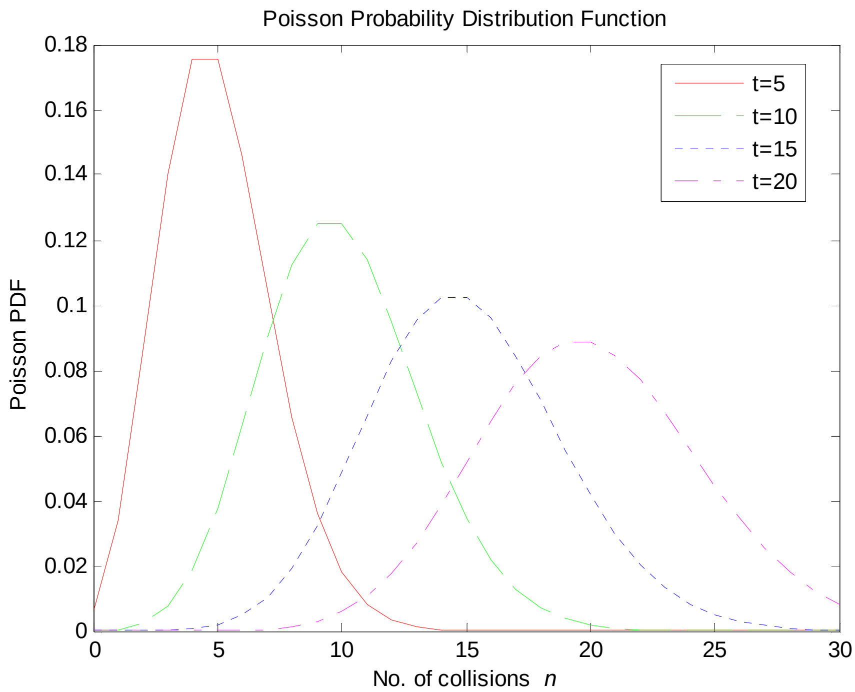

Figure-8. Poisson probability distribution function (PDF).

CONCLUSIONS

The collision density and transmission probability were estimated for monoenergetic transport of radiation in a 1-D slab with forward scattering. Two estimators *viz* the collision estimator (CE) and the track-length estimator (TLE) were used and the number of collisions were tallied for the histories, to construct a PDF for the events. It was found that the CE is valid only when the region dimensions are larger than the optical distance and for such cases only the TLE can give a reliable result. The constructed PDFs were compared with the Poisson PDF and good agreement was obtained. The simulation was shown to be equivalent to the iterative process in the solution of the governing integral equation which models radiation transport in matter.

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