Simulating optical processes: Monte Carlo *photon* tracing method

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В поисках высокой точности и практической реализации вычислительная оптика использует несколько методов моделирования, такие как методы, основанные на уравнениях Максвелла, метод трассировки лучей, методы оптики Фурье и т. д. Каждый из этих методов имеет свои преимущества, недостатки и ограничения применимости. В этой статье мы описываем отслеживание фотонов методом Монте-Карло как метода моделирования в вычислительной оптике. Обоснованность основных допущений в используемом методе моделирования продемонстрирована на примерах. Обсуждаются ограничения применимости метода.

Ключевые слова: фотон, метод Монте-Карло, оптические поля, симуляционная модель

In search of high accuracy and convenient implementation, computational optics uses several modeling techniques such as Maxwell's equations-based methods, ray-tracing method, Fourier optics methods and many others. Each with its advantages, disadvantages, and applicability caveats. In this paper, we describe Monte Carlo *photon* tracing as a simulation technique for computational optics. The validity of the main assumptions in the simulation method is demonstrated with examples, and limitations of method's applicability are discussed.

Keywords:photon, Monte Carlomethod, optical fields, simulation model.

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I. Introduction

Advances in the field of applied science ranging from microorganisms to astronomical studies occur due to, along with many other factors, the availability of accurate and user-friendly models. Indeed, today's computing capabilities to understand and solve complex problems have become essential in scientific research and economics, military, and social science [1]. It is reasonable to assume that the first step in the emergence of new technology, be it a medical diagnostic tool or scientific equipment, starts with modeling physical processes. For that matter, developing convenient, cost-effective and accurate modeling methods is considered a critical and high-yielding study. In the literature, it is accepted that there are two families of models: scientific (mathematical) and statistical. Scientific models are presumably accurate because they are usually derived from fundamental equations such as Maxwell and Schrödinger. In practice, however, scientific models make use of several approximations to achieve closed-form formulation or solvability [2],resulting in degraded accuracy. Statistical models rely in part on randomness (statistical laws) to determine a "highly probable outcome" at the expense of less precision. A famous example of using a statistical model is estimating the likelihood that the chain reaction required for an atomic bomb would work successfully. Problems and issues discussed in this manuscript relate to the latter.

Maxwell's equations (MEs) are the starting point in developing any formulation and model in optics and photonics [3]. MEs-based methods deserve high praise for their mathematical rigor, scientific

elegance, and accuracy. For example, models built on solutions of MEs by finite-difference time-domain method [4] theoretically can be applied to any system. However, despite the fact that these methods have been around for more than four decades, they did not find widespread utility in optics and photonics. One possible explanation is that complexity of a system makes it conceptually and computationally too tricky. That is, the adaptation of system parameters into a model becomes impractical, requiring extra effort. On the contrary, methods like ray tracing of geometrical optics, despite apparent limitations, are used by the majority in optical engineering due to their simplicity and intuitiveness. Several ready-to-use ray-tracing-based software packages (such as LASCAD and ZEMAX) have been offered and widely used commercially. However, ray tracing methods are inapplicable for modeling optical systems governed by the principles of wave and electromagnetic optics [5].

Thus, on the one hand, we have mathematically rigorous methods based on MEs, which are not easy to apply to complex optical systems. On the other hand, quickly implementable methods, such as ray tracing, are applicable only in geometric optics. The Monte-Carlo photon tracing (MCPT) technique was developed as an alternative to the ray-tracing method. Previously, MCPT was successfully used to design and optimize solar pumped lasers [6-8]. MCPT details are scattered on several papers. However, the full model description of MCPT has not been given so far. Therefore, we describe Monte Carlo photon tracing, demonstrating each step in detail. Before everything, the photon concept must be stressed that we are not considering the quantum photon with its duality properties. We consider that the optical field consists of point-like entities with distinguishing physical properties, called *photons* in the text.

II. Photon tracing

In general, model hardware in optics consists of an illumination source to generate an optical field, an optical system with which the field interacts, and a detector where the field is registered.

An optical field generated by any source is described mainly by its spatial, temporal, and spectral characteristics. In addition, the optical field has directivity, coherence, and polarization properties, although these properties are all interrelated. Here, we present a basic formulation of how some of these properties are adapted into a model by MCPT.

Spatially-dependent characteristics. Optical fields generated from illumination sources have complex spatial features from sunlight to structured optical fields [9]. A common approach for coping with complex beams is decomposing the optical field into elementary entities like rays or plane waves [10]. Following this methodology, MCPT views an optical field as the sum of particles and can be called *photons* with specified spatial coordinates. An underlying reason for the *photons* assumption will become clear later in the text.

Since our previous studies were only concerned with solar photons, MCPT models so far could consider directionality and spectral characteristics. For the case of solar radiation, the decomposition of the illumination source is straightforward because, at the observation plane (or starting point of a model), solar photons have the same directionality property and uniform intensity distribution. In other cases, however, the situation is different. As an example, consider a Gaussian beam, the propagation of which is plotted in Fig. 1 using the following complex amplitude equation [5]:

$$E(\vec{r}) = E_0 \frac{W_0}{W(z)} \exp\left[\frac{\rho^2}{W^2(z)}\right] \exp\left[-jkz - jk\frac{\rho^2}{2R(z)} + j\xi(z)\right] \quad (1)$$

where $W_0 = \sqrt{\lambda z_0 / \pi}$ is the beam waist, $W(z) = W_0\sqrt{1+(z/z_0)^2}$ and $R(z) = z\left[1+(z/z_0)^2\right]$ are measures of the beam width and wavefront radius of curvature, $\xi(z)$ is phase retardation.

From Fig. 1, it is noticeable that as the Gaussian beam propagates, its intensity profile radially spreads.

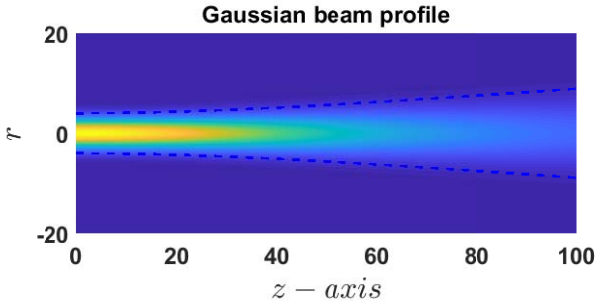


Figure 1. Gaussian beam.

To account for the spatial variance of the Gaussian beam profile in the context of MCPT, the intensity distribution at the waist can be used as a probability density function to draw sample photons with

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specified coordinates. This assumption is justified because the intensity is related to the population of photons in a given volume, that is, the irradiance is linearly proportional to the number of photons per unit volume, $I = (n/V)hc^2/\lambda$.

The divergence cone with a maximum angle $\theta = \lambda/(\pi W_0)$ can be used to determine the directions of initialized photons. By considering the parameters used in plotting the Gaussian beam profile in Fig. 1, we simulated the propagation of the Gaussian beam, decomposing it into photons, as depicted in Fig. 2.

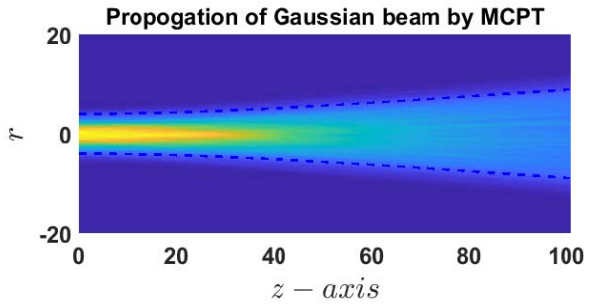


Figure 2. Simulation of Gaussian beam propagation via MCPT.

These two graphs show good agreementbesides minor smoothness, demonstrating representative power of the *photons* expansion method. In this manner, the decomposition of an arbitrarily shaped optical beam into *photons* is easily achievable using the beam parameters. In addition, the ray-based approach methods pioneered by Miguel A. Alonso and his colleagues to construct structured optical beams [11-13] can be adapted.

Spectral characteristics. In a similar way to the spatial case, the optical spectrum $S(\lambda)$ of a source serves as a probability density function for determining the wavelength of photons. The wavelength is considered as a random variable with non-uniform probability density defined as

$$f(\lambda) = \frac{S(\lambda)\frac{\lambda}{hc}}{\int_0^\infty S(\lambda)\frac{\lambda}{hc}d\lambda}, \quad (2)$$

so that the following condition satisfies

$$\int_0^\infty f(\lambda)d\lambda = 1. \quad (3)$$

Then, the wavelength λ is determined by numerically solving the following integral equation:

$$\xi = \int_0^\lambda f(\lambda')d\lambda', \quad (4)$$

where ξ is the random number uniformly distributed over [0,1]. To illustrate, we used the AM1.5 solar radiation spectrum to initialize solar photons with specified wavelengths. Figure 3 shows a comparison of the solar spectrum and the aggregated spectrum of initialized photons with different numbers of photons. The accuracy of spectrum approximation (fitting) improves with an increased number of photons (Fig. 3b).

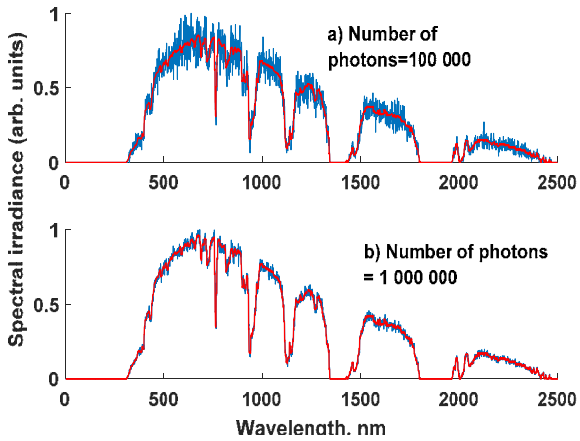


Figure 3. a) Red line is the solar spectrum, the blue line is the aggregated spectrum randomly initialized solar photons with 100 000 photons, b) The case with 1 000 000 photons [8].

III. The optical system

An arbitrary optical system can have several elements with distinct optical properties. In MCPT, the interaction of photons with matter is formulated through macroscopic properties like the refractive index of the medium, surface reflectivity, transmission (transparency), absorption, and emission spectrum.

The intersection of a photon with matter. As in the ray-tracing method, a photon initialized from a source with specified coordinates $\boldsymbol{r}(x,y,z)$ and direction cosines $\boldsymbol{\upsilon}(\upsilon_x, \upsilon_y, \upsilon_z)$ points toward the matter surface (Fig. 4).

The intersection point of the travelling photon with a surface and the distance are determined from the surface equation, the initial coordinates of the photon, and the direction cosines. Then, the photon has to propagate to the point, which ends the similarity between ray tracing and photon tracing.

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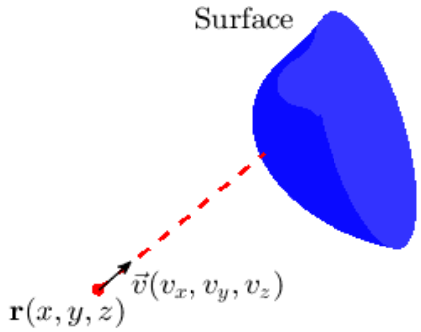


Figure 4. The photon-surface intersection.

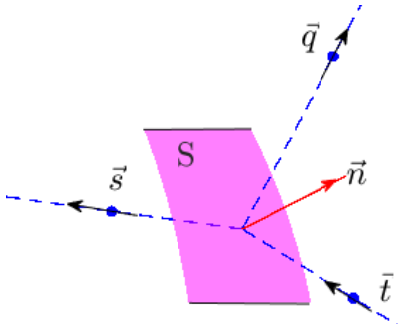


Figure 5. Processes at the boundary.

The interaction. On the surface, the quantum nature of the photon is taken into account: since the photon with a direction $\vec{t}$ cannot be split, it must be reflected $\vec{q}$ or refracted $\vec{s}$ at the boundary (Figure 5). These directions can easily calculate:

$$\vec{q} = \vec{t} - 2(\vec{t} \times n)\vec{n}$$

$$\vec{s} = \frac{n_1(\vec{t} + \vec{n}(\vec{t} \times \vec{n}))}{n_2} - n\sqrt{1 - \frac{n_1^2(1-(\vec{t} \times \vec{n})^2)}{n_2}} \,. \quad (6)$$

The likelihood of one of two possible scenarios is determined from the state of polarization, the angle of incidence, and the normal to the surface. This is the key difference between photon tracing the traditional ray tracing. To illustrate, one can consider a simple optical system that consists of three optical elements: quartz, a conical reflective surface, and a crystal (Fig. 6).

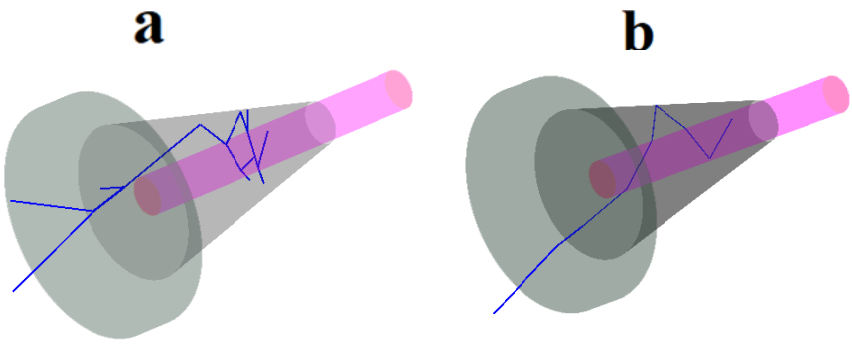


Figure 6. Demonstration of ray (a) and photon (b) tracing.

In the case of Fig. 6a, the ray split into two at each interface between two media, and even with some simplifications, after 4-5 interactions with optical elements, as a result of this branching, one individual ray split into seven rays. In this way, the number of "newly-born" rays increases exponentially. If one considers an optical beam and a complex optical system, the number of rays in the system becomes enormous, and tracing each of them becomes a challenging task that requires enormous computing power. Fig. 6b illustrates the photon tracing method. Here, we do not observe "the branching". Therefore, the photons assumption greatly simplifies simulating optical processes that can be executed using moderate PC power.

Absorption of a photon by medium. When photons propagate in a medium, they might get absorbed,that is photon annihilation may occur. This can be modeled via the absorption spectrum,one of the optical mediums' main characteristics. In addition, the techniques used in the experimentally validated Monte Carlo method for photontransport simulation can be adapted [14,15]. Thus, the absorption length *l*(the distance the photon travels until it is absorbed) can be derived from the inverse distribution method and the Beer-Lambert law:

$$l = -\ln \xi / \eta \,, \quad (7)$$

where ξ is a random number and η is the absorption coefficient for the given wavelength. For demonstra-

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tion, one can examine the absorption of a Gaussian beam with two different wavelengths 530 nm and 807 nm in Nd:YAG crystal (Fig. 7). As shown in Fig. 6, photons with these two wavelengths have two different absorptioncoefficients in the Nd:YAG. As a result, the absorption distributions should be distinct for each case (Fig. 8).

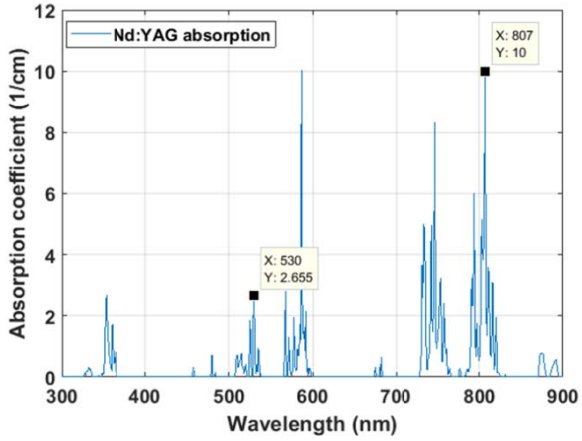


Figure 7. The abruption spectrum of Nd:YAG.

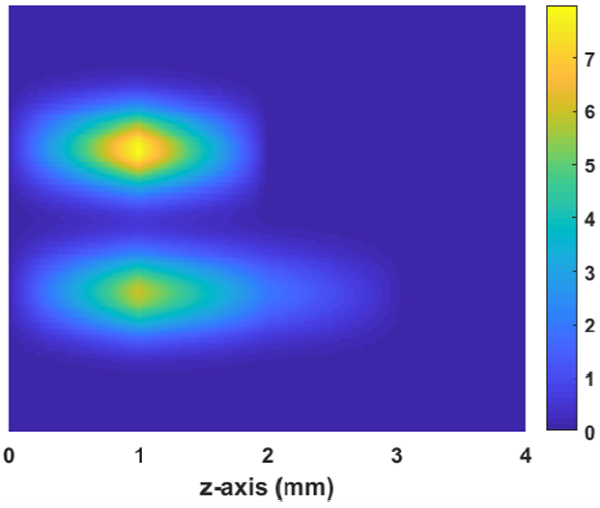


Figure 8. The absorption distributions of Gaussian beams in Nd:YAG.

Creation of a photon in a medium. After the photon annihilation in the medium, the absorbed energy triggers the subsequent process. For example, the energy can give rise to the temperature of the medium. More important to our study is that the energy causes a new photon to be created. That is, the emission process occurs. So, the emission spectrum of the medium is exploited to model the creation of the new photon, where the absorption point of the old photon is used as the coordinates of the newly initiated photon. The direction cosines are updated by arbitrary values taken within 4π due to the physics of the spontaneous emission process unless a stimulated emission occurs.

IV. Detecting photons

The detection or registration of a photon is a delicate matter that is not entirely formulated even in the quantum optics framework [16]. Therefore, we know that discussing this issue in the MCPT framework seems pointless. However, for our simulation purposes, we are using a simple procedure: the observation plane, for example, it can be the surface of the detector. The surface is gridded in two dimensions (x-y), and each grid counts incident photons with their energies:

$$E = h\nu_1 + h\nu_2 + \ldots + h\nu_n . \qquad (8)$$

In addition to, the photon detection, using this procedure, 3D photon distributions can be obtained and further used to calculate power, intensity, irradiance and energy distributions.

V. Discussions

Models based on MCPT give excellent accuracy for experiments involving sources, which produce random optical fields (not monochromatic, not coherent and unpolarized). Solar radiation can be an excellent example of this kind of source. Recently, we tested MCPT for experiments with light-emitting diodes, and initial results showed encouraging signs [17]. MCPT can be very useful for complex optical systems. For example, biological mediums are not easy to model [18] because of their structural complexity.

The main limitation of MCPT is that it cannot simulate the interference (diffraction) processes, which are present in most cases if one works with monochromatic sources. That is, the wave nature of the optical fields is mainly ignored. However, most experiments in modern physics involve lasers, which means a new model should consider the interference process to achieve high accuracy. The same can be stated for optical engineers' well-established ray tracing method. Another limitation is that MCPT does not consider the polarization of electromagnetic fields so far, and this is hugely important in electromagnetic optics. In recent years, studies on vortex beams and optical tweezers increased the importance of the polarization in emerging optical technologies [19].

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VI. Conclusions

We describe the Monte Carlo *photon* tracing method in detail. Its validity and usefulness in computational optics are demonstrated, and applicability caveats and limitations of MCPT are discussed. Currently, we are conducting studies to modify MCPT with additional features to account for interference and polarization to widen application areas.

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Оптик жараёнларнинг симуляцияси: Монте Карло фотон трассировка методи

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Оптикада юқори аниқлик ва амалийликни таъминлашда бир неча моделлаштириш усулларидан фойдаланади, масалан, Максвелл тенгламаларига асосланган усуллар, нурларни кузатиш, Фурье оптикаси усуллари ва бошқалар. Ҳар бирининг ўзига хос афзалликлари, камчиликлари ва чекловлари мавжуд. Ушбу мақолада оптик жараёнларни симуляциялаш учун Монте-Карло фотон трассировка методи тавсифи келтирилган. Моделлаштириш методидаги асосий ёндашувлар ва фаразларнинг асосланганлиги мисоллар билан кўрсатилди. Усулнинг қўлланилиш чекловлари муҳокама қилинди.

Калит сўзлар: фотон, Монте-Карло методи, оптик майдон, симуляцион модел.

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