Fast Perturbation Monte Carlo simulation for heterogeneous medium and its utilization in functional near-infrared spectroscopy

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Abstract. In near-infrared spectroscopy, fiber optic probe is usually applied to incident light into the bio-sample and detect the spatial and temporal resolved optical signal re-emitted from the turbid medium. In this point-source-point-detector measurement system, seed Perturbation Monte Carlo (Pmc) method is an effective model to perform the forward simulation. In our study, the integration of parallel computing with graphics processing units (GPU) into the existing seed Pmc method substantially accelerate the speed of the original simulation. The GPU based seed Pmc provide an excellent solution for the application of fiber optic probe in both homogeneous and heterogeneous turbid medium.

1. Introduction
The forward model for simulating light migration in turbid sample is mainly based on the radiative transport equation (RTE) [1]. In practice, when $\mu_s \gg \mu_a$ and the source is far away from the detectors, diffusion approximation can be introduced into RTE to derive the diffuse reflectance or transmittance more effective [2]. However, in fiber optic probe to interrogate bio-sample, in order to manufacture a small probe, the incident fiber is assembled side by side next to the detection fiber. [3] Furthermore, for some special fiber optic probe, it is hard to concern the complex boundary condition between the probe and the tissue sample. Monte Carlo simulation offers a flexible method based on tracing photon emitted from fiber and propagating in turbid medium. Therefore in MC simulation, the fiber optic probe can be designed in arbitrary geometric structure [3] and placed on arbitrary position of the turbid medium. But this method is statistical in nature and it must trace a large number of photons to reduce the statistical error. Alex et.al. have introduce GPU to accelerate MC simulation and gain 1000 speeded-up compared with a traditional CPU based program. Ref [5] indicates that for a point-source-point-detector measurement system (i.e. fiber optic probe), the vast majority of photons do not contribute to the detection result because the detection rate is limited by the diameter of fiber core. Hence, a new sampling method (i.e. seed Perturbation Monte Carlo (Pmc)) can be introduced to improve the efficient of MC simulation for fiber probe system. The seed Pmc records the detected photon and abandon the other photons during its first step. Once the valuable seeds for the detected photons are recorded, they can be used in the second-step of seed Pmc simulation to effectively

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calculate the diffusive reflectance or transmittance. The less the ratio of the detected photons to the total simulation photons is, the more effective the seed Pmc model will be. However, the photon trajectory is determined by the scattering coefficient, in order to perform the seed Pmc within large range of scattering coefficients, it needs to record the valuable seeds by running the first-step seed Pmc with the corresponding scattering coefficients. It’s worth to mention that the absorption coefficient can be varied arbitrarily in the second-step.

In our previous work [6], we have applied the seed Pmc model in GPU program and verify that the seed Pmc model has the ability to calculate the diffuse transmittance with various scattering coefficient in point-source-planar-detector system. In the present study, the similar simulation program will be used in the point-source-point-detector measurement system. The traditional MC and seed Pmc are all performed by using GPU, and the seed Pmc is at least 1000 factor faster than MC. Last, the brain model will be utilized in the seed Pmc method. The result demonstrates that the seed Pmc can also generate the Time domain reflectance more effectively.

2. Two-step seed Pmc to solve RTE with arbitrary scattering and absorption coefficients

Fiber optic probe provides a flexible solution for an optical platform between the spectroscopic device and the sample to be interrogated in situ. The illumination and detection fibers are usually separate to improve the system SNR [3]. To minimize the size of the probe, the separation of the illumination and detection fiber must be small enough. In this case, the diffusion equation is failed to calculate the reflectance result. In our study, the seed Pmc is consider to simulate the spatial resolved reflectance of fiber optic probe with fibers cling to each other. The seed Pmc can be described as two-step MC simulation, as shown in Fig.1. The main procedure of simulation of photon in the heterogeneous medium is according to Ref [7]. The voxels size is 1 mm. In the first-step Pmc, a GPU (NVIDIA® GeForce® GT 240M) is used to perform the MC for fiber-based detection and record the valuable seeds in the computer disk. Here, the valuable seeds can ‘move’ the photons from the source fiber into the turbid sample and backscatter into the detection fiber. The valuable seeds can only work for a given scattering coefficient. Hence the first step will be run for 100 times for scattering coefficient varied from 1cm⁻¹ to 100cm⁻¹ to derive and store the corresponding valuable seeds. Note that, the medium is heterogeneous here, the scattering coefficient for all voxel is set as the same value and the absorption coefficient can be set as arbitrary value for each voxel. Then, the valuable seeds can be applied in the second-step Pmc to generate the diffusive reflectance with a large range of scattering coefficient (1cm⁻¹ to 100cm⁻¹, the value of scattering coefficient must be integer between 1-100) and arbitrary absorption coefficient. The first-step Pmc is just performed to record the valuable seeds and the second-step Pmc is the mainly procedure to calculate the reflectance for various scattering and absorption coefficients, therefore in the following only the running time of second-step Pmc is recorded.
3. Simulation of spatial resolved reflectance by fiber optic probe

A simple fiber reflectance probe is simulated in this study to demonstrate the ability of the seed Pmc. As shown in the inset of Fig.2(b), five-fibers are placed on the tissue to illuminate the sample and pick up reflectance light. This fiber probe has been used widely in tissue detection to obtain the scattering and absorption coefficients of turbid medium according to the reflectance. [3] The turbid medium is set as homogeneous turbid sample in this case. The fibers in the probe have 200 μm core and 300 μm cladding. The numerical aperture is 0.22. In order to overcome the statistical error, the stop criterion for MC and seed Pmc is that the fibers 2-4 pick up to 40000 reflected photons during the simulation. Fig.2(a) illustrates the reflectance of fibers 3-5 according to different scattering coefficients. It’s worth noting that the sampling method in the seed Pmc is based on the valuable seeds (i.e. all simulated photons will be detected by the detected fibers in the second-step Pmc.), so the absolute reflectance of the fiber optical probe cannot be derived. In Fig.2(a), F3-F5 are the reflectance of fibers 3-5 which are normalized by reflectance of fiber 2. The absorption coefficient and the anisotropy factor are set as 0.01 mm⁻¹ and 0.8 respectively. The relative error between PMC and traditional MC is shown in the inset of Fig.2(a). The speedup factors are illustrated in Fig.2(b). To detect 40000 photons by fibers 2-5, it up to takes 0.06 second to finish the second-step Pmc.
4. Simulation of temporal resolved reflectance in functional near infrared spectroscopy

Furthermore, the seed Pmc can be applied in heterogeneous brain medium. Herein the voxel-based anatomical model of human head [8] is used. The input light wavelength is 632 nm and the optical coefficients of the skin, skull, white matter, grey matter and CSF are obtained from [8]. In functional near infrared spectroscopy (fNIRS) [9], fibers are usually exploited as transceiver to monitor the blood concentration of cerebral cortex. A schematic diagram is shown in Fig.3(a). One fiber is placed on the top of the head to incident a 632 nm laser into the head and another fiber, which is 1 cm apart from the first one, is utilized to measure reflectance light in time-domain. Two-dimensional representation of the distribution of optical intensity is shown in Fig.3(a), which illustrates that the 632 nm laser can penetrate the skull and arrive the brain region. Besides, seed Pmc is capable of calculating the temporal resolved reflectance in the head model. In the temporal resolved seed Pmc, the length of the photon’s trajectory is recorded during the simulation and contributes to different time frame. The seed Pmc proves to be about 3000 factor faster than traditional MC. As mentioned before, the use of seed

Figure 2. (a) The normalized spatial resolved reflectance of fiber 3-5 with different scattering coefficients. (b) The speed-up factor compared with seed Pmc and traditional MC simulation.
Pmc simulation is more accurate and convenient than diffusion equation, which is mainly used at present, hence seed Pmc holds great potential to become a better forward model to solve the change of the scattering and absorption coefficients due to the brain activity [9].

![Figure 3](image_url)

**Figure 3.** (a) The distribution of optical intensity inside a human head. A fiber is used to input the light into the head, and another fiber, which is 1 cm apart from the source fiber, is used to take the temporal resolved signal, as shown in (b). The perform time for derive the temporal resolved signal by MC and seed Pmc is 62369 second and 20.88 second respectively.

5. Conclusions
All of the seed Pmc simulation is performed on a laptop computer with a modest GPU (GT 240M). Even so, the seed Pmc behaves much better than the traditional MC model. In fiber optical probe (the inset of Fig.2(b)), it only takes about 0.06 second to generate the simulation result. Also, the seed Pmc can handle an arbitrarily complex medium, such as the human head and also gains a remarkable speedup compared with MC model. As mentioned above, the seed Pmc can deal with a sample with complex boundary condition as the traditional MC model does. By using an advanced GPU or Scalable Link Interface(SLI) to combine several modest GPU, this seed Pmc model has the realistic ability, rather than the potential, to realize real-time forward simulation for light migration in turbid medium with a point-source-point-detector system.

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