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Accelerated modeling of light transport in heterogeneous tissues using superposition of virtual sources

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ABSTRACT

We present a perturbation theory for diffusive light transport in turbid media, which allows to model the light distribution around inhomogeneities of complex geometries. The diffusion equation for an inhomogeneous medium is transformed into an equivalent integral equation that can be solved with a fast iterative numerical algorithm. This method models three dimensional geometries considerably faster than standard methods. Furthermore, the integral formulation supports an intuitive understanding of the physical processes.

1. INTRODUCTION

Modeling the light distribution in heterogeneous tissues is a key to the successful use of light in medicine. For clinical applications, especially for inverse problems in imaging, it is desirable to model complex three dimensional geometries *fast.* An important class of problems can be described as an otherwise homogeneous host or background medium containing perturbing objects of different optical properties. Examples are buried tumors or blood vessels in tissues. Several methods have been used to solve this kind of problems, but computation time remains a problem. Monte Carlo simulations[1] are principally accurate but very slow, because a large number of photons need to be traced to get a reasonable variance far away from the source. Finite Element[2] or Finite Difference[3] methods solve the differential diffusion equation on a grid that has to cover all sources and objects. If the geometry has to be modeled in three dimensions, this leads to a large number of grid elements and therefore high computation cost.

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Our approach is not to solve the differential diffusion equation, but its equivalent integral equation. An advantage of this formulation is that it starts from the known solution for the unperturbed homogeneous host medium and thus uses a priori information. The integral equation then determines the perturbation of the light field due to the objects and has to be solved *only in the volume of the perturbing objects*. After the light distribution in the objects is calculated, the light field at any other location, e.g. at a detector, can be obtained by a simple integration over the objects.

The aim of this paper is to introduce the approach in its simplest form. We therefore restrict ourselves to the steady state case and inhomogeneities having different absorption coefficient than the background medium.

2. DIFFUSION EQUATION

For steady state problems, the P1 approximation of the radiative transport equation yields the time independent diffusion equation[4,2]:

$$\nabla\big(D(\mathbf{r})\nabla\phi(\mathbf{r})\big) - \mu_a(\mathbf{r})\,\phi(\mathbf{r}) = -S(\mathbf{r}), \tag{1}$$

where $\phi(\mathbf{r})$ is the light fluence, $\mu_a(\mathbf{r})$ is the absorption coefficient, $\mu_s'(\mathbf{r})$ is the reduced scattering coefficient, $D(\mathbf{r}) = 1/[3(\mu_a(\mathbf{r})+\mu_s'(\mathbf{r}))]$ is the diffusion coefficient, and $S(\mathbf{r})$ is the source function. In most biological tissues the strong scattering condition, $\mu_s'(\mathbf{r}) >> \mu_a(\mathbf{r})$, is satisfied. The diffusion coefficient can then be approximated as $D(\mathbf{r}) \approx 1/(3\mu_s'(\mathbf{r}))$. This means that for the case of an object with different absorption but the same scattering coefficient than the background medium, the diffusion coefficient $D(\mathbf{r}) = D_0$ is a constant. Equation (1) is then simplified to

$$\nabla^2\,\phi(\mathbf{r}) - \frac{\mu_a(\mathbf{r})}{D_0}\,\phi(\mathbf{r}) = -\frac{S(\mathbf{r})}{D_0}\,. \tag{2}$$

We split the absorption coefficient into a constant background part and a perturbation part

$$\mu_a(\mathbf{r}) = \mu_{a0}+\Delta\mu_a(\mathbf{r}). \tag{3}$$

This allows to write eqn.(2) as a perturbed Helmholtz equation

$$\left(\nabla^2 + k^2\right)\phi(\mathbf{r}) = -\frac{S(\mathbf{r})}{D_0} + \frac{\Delta\mu_a(\mathbf{r})\phi(\mathbf{r})}{D_0}, \tag{4}$$

where $k^2 = -\mu_{a0}/D_0$ accounts for the background optical properties. The influence of the inhomogeneities has thus been confined to a single term. Now we transform the differential equation (4) into an equivalent integral equation.

3. TRANSFORMATION OF THE PERTURBED HELMHOLTZ EQUATION INTO AN INTEGRAL EQUATION

We first return to the unperturbed Helmholtz equation for the homogeneous medium in order to show how the Green's function links the differential to the integral equation. The Green's function $G(|\mathbf{r}-\mathbf{r}'|)$ of the Helmholtz equation is defined as the solution for a mathematical point source at $\mathbf{r}'$

$$\left(\nabla^2 + k^2\right) G(|\mathbf{r}-\mathbf{r}'|) = -\delta(\mathbf{r}-\mathbf{r}'). \tag{5}$$

For three dimensions the Green's function is

$$G(|\mathbf{r}-\mathbf{r}'|) = \frac{1}{4\pi\,|\mathbf{r}-\mathbf{r}'|}\, e^{ik(|\mathbf{r}-\mathbf{r}'|)}. \tag{6}$$

For the unperturbed homogeneous background medium, the solution $\phi_0(\mathbf{r})$ for an arbitrary source distribution $S(\mathbf{r})$ can be easily obtained as a convolution of the source function $S(\mathbf{r})$ with the Green's function:

$$\phi_0(\mathbf{r}) = \int_V d\mathbf{r}'\, S(\mathbf{r}')\, \frac{G(|\mathbf{r}-\mathbf{r}'|)}{D_0}. \tag{7}$$

This is in fact the equivalent integral equation for the Helmholtz equation without perturbation term.

By analogy, for the perturbed Helmholtz equation (4) the integral equation is

$$\phi(\mathbf{r}) = \int_V d\mathbf{r}' \left(S(\mathbf{r}') - \Delta\mu_a(\mathbf{r})\phi(\mathbf{r})\right) \frac{G(|\mathbf{r}-\mathbf{r}'|)}{D_0} \tag{8}$$

or $$\phi(\mathbf{r}) = \phi_0(\mathbf{r}) - \int_{V_{obj}} d\mathbf{r}'\, \Delta\mu_a(\mathbf{r})\, \phi(\mathbf{r})\, \frac{G(|\mathbf{r}-\mathbf{r}'|)}{D_0} . \tag{9}$$

The formal derivation[5] is outlined only briefly: we multiply equation (4) from the left with $G(|\mathbf{r}-\mathbf{r}'|)$, multiply eqn. (5) from the left with $\phi(\mathbf{r})$, then subtract eqn. (4) from (5) and integrate the resulting equation over the whole space. We use Green's theorem to transform the volume integral over the derivatives into a surface integral:

$$\int_V d\mathbf{r}'\left[\phi(\mathbf{r})\nabla^2 G(|\mathbf{r}-\mathbf{r}'|) - G(|\mathbf{r}-\mathbf{r}'|)\nabla^2\phi(\mathbf{r})\right] = \int_{S(V)} d\mathbf{A}'\left[\phi(\mathbf{r})\nabla G(|\mathbf{r}-\mathbf{r}'|) - G(|\mathbf{r}-\mathbf{r}'|)\nabla\phi(\mathbf{r})\right] . \tag{10}$$

The surface integral vanishes since the surface extends to infinity and the Green's function decays exponentially. This finally yields integral equation (9), which is strictly equivalent to the differential diffusion equation (2).

4. SOLUTION OF THE INTEGRAL EQUATION WITH PERTURBATION THEORY

If the effect of the perturbation is expected to be small and consequently the solution $\phi(\mathbf{r})$ is similar to $\phi_0(\mathbf{r})$, equation (9) can be approximated by using the unperturbed solution ϕ_0 in the integral. This yields a first order approximation ϕ_1, which is commonly known as the Born approximation. In general, higher approximations of n-th order can be obtained iteratively with the following recursion formula:

$$\phi_n(\mathbf{r}) = \phi_0(\mathbf{r}) - \int_{V_{obj}} d\mathbf{r}'\, \Delta\mu_a(\mathbf{r})\, \phi_{n-1}(\mathbf{r})\, \frac{G(|\mathbf{r}-\mathbf{r}'|)}{D_0} . \tag{11}$$

Noting that $S\cdot G(\mathbf{r}|\mathbf{r}') / D_0$ describes the fluence due to a point source of strength S at $\mathbf{r}'$ in the homogeneous background medium, this result may be interpreted as follows. At each infinitesimal volume element $dV'=d\mathbf{r}'$, a *virtual source* emits light which is superimposed to the background light field. The source strength of this virtual source is $S = -\Delta\mu_a(\mathbf{r}')\, dV'\, \phi(\mathbf{r}')$ which is the additional absorbed power in this volume element, caused by the absorption perturbation. Thus the virtual source re-emits the additional absorbed light with the opposite sign. The intuitive interpretation is that an object with increased absorption 'sucks out' light from the surrounding, while an object with decreased absorption acts like producing light. The iteration scheme in eqn. (11) reflects the counteraction of the voxels by shadowing each other.

For numerical evaluation, the inhomogeneities are divided into small voxels of volume ΔV, and the integral is approximated as a sum over those voxels. The solution is a two step process. First, the fluence at the center points $\mathbf{r}_j$ of the voxels is determined iteratively. It is convenient to write the fluence and the absorption coefficient at these points as vectors $\phi_n[j]$ and $\Delta\mu_a[i]$, and the Green's function $G(|\mathbf{r}_j - \mathbf{r}_i|)$ as a matrix G_{ji}. Note that for i=j, the Green's function $G(|\mathbf{r}_j - \mathbf{r}_i|) = G_{ji}$ has a singularity. We therefore use the spread function of a spherical distributed source whose radius R is chosen so that its volume matches the volume of the voxels. The modified Green's function for the center of such a source is

$$G_{jj} = \frac{-3}{4\pi k^2 R^3}\left(1-(1-ikR)e^{ikR}\right) \tag{12}$$

Defining a transfer matrix $T_{ij} = \Delta V\ \Delta\mu_a[i]\ G_{ji} / D_0$, the discrete version of equation (11) can be written in matrix form

$$\phi_n[j] = \phi_0[j] - \sum_i^{\text{voxels}} T_{ij}\, \phi_{n-1}[i]\ . \tag{12}$$

The algorithm for the iteration is then:

calculate $\phi_0[j]$ for all voxels j;

n=0;

do{

n=n+1;

for all j do: $\phi_n[j] = \phi_0[j] - \sum_i^{\text{voxels}} T_{ij}\, \phi_{n-1}[i]$;

} while maximum change $|\ \phi_n[j] - \phi_{n-1}[j]\ |$ is greater than a threshold.

Once the fluence $\phi_n[j]$ at the voxels in the objects has been obtained, the second step is to calculate the fluence at any desired position $\mathbf{r}^*$ by a single summation

$$\phi(\mathbf{r}^*) = \phi_0(\mathbf{r}^*) - \sum_i^{\text{voxels}} \Delta V \, \Delta\mu_a[i] \, \phi_n[i] \, \frac{G(|\mathbf{r}^* - \mathbf{r}_i|)}{D_0} \,. \tag{13}$$

5. EXAMPLES

In order to test our approach, we compared it with two other methods: Monte Carlo simulation[7] and a solution of the differential diffusion equation. For simple geometries it is possible to solve the diffusion equation with a boundary condition method. Therefore, we chose a simple test geometry: a sphere with increased absorption in an otherwise homogeneous background medium,

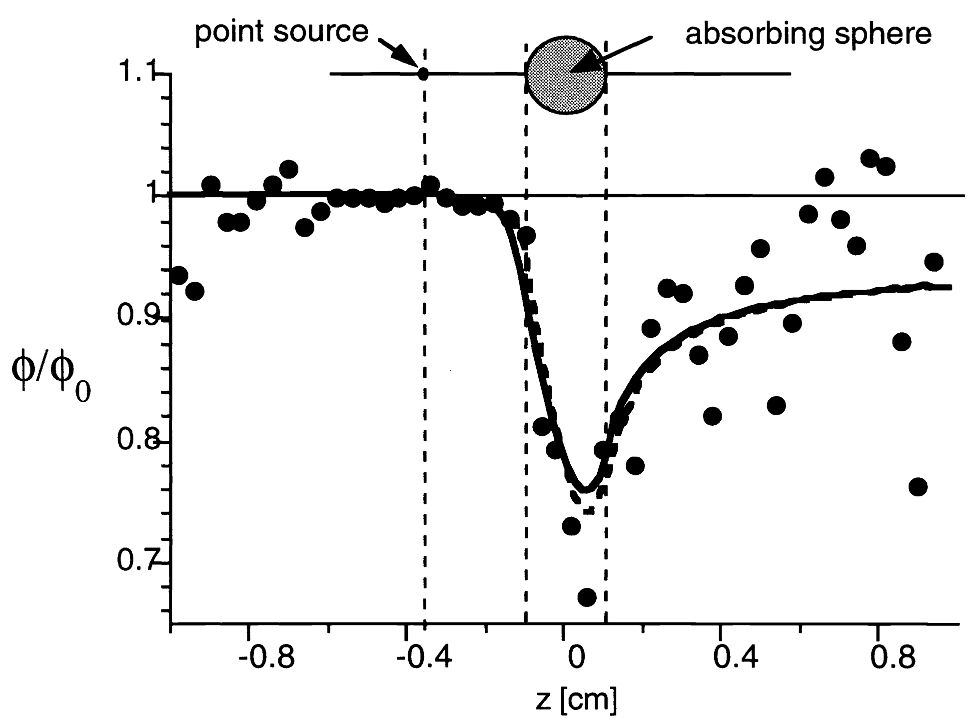

Figure 1: Comparison of the perturbation theory method (solid line) with a spherical harmonics expansion (dashed line) and Monte Carlo simulation (dots). The normalized fluence on a line through the center of a sphere and the source has been plotted. The optical properties of the background medium are $\mu_a = 1$ cm^{-1} and $\mu_s' = 12$ cm^{-1}, the sphere has $\mu_a = 3$ cm^{-1} and $\mu_s' = 12$ cm^{-1}. For the perturbation theory method the sphere has been modeled with 81 virtual sources.

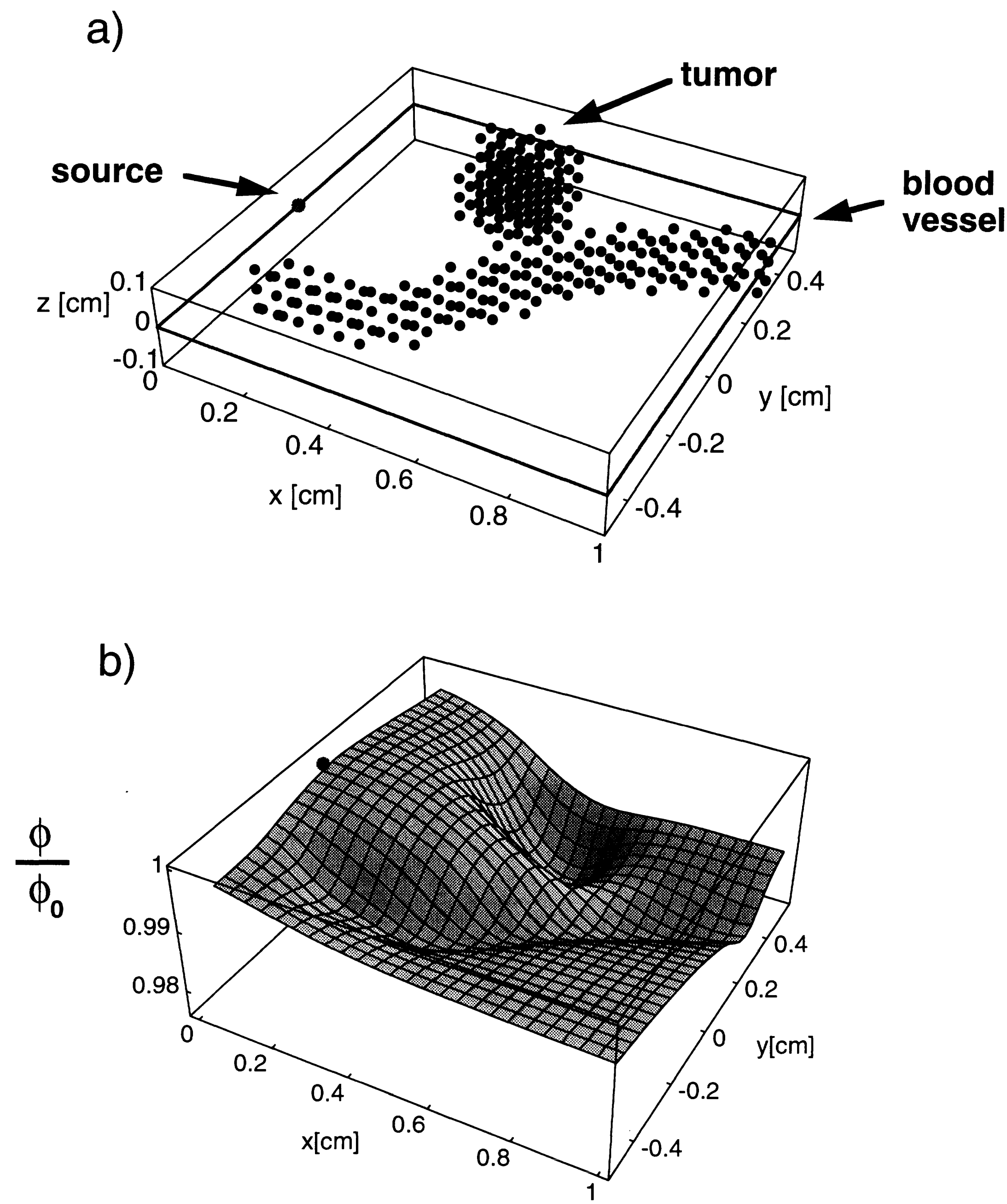

Figure 2: Example for a complex geometry. The optical properties of the background are μ_a $=0.1$ cm^{-1} and $\mu_s'=10$ cm^{-1}, the objects have the same scattering and doubled absorption. The objects have been approximated with 266 voxels. The points in picture a) represent their center points. Picture b) shows the fluence ϕ in the plane through the illuminating primary source and the objects, normalized to the background fluence ϕ_0. The computation time was five seconds on a Sun SPARCstation 10 for five iterations.

irradiated by an isotropic point source. For this geometry it is possible to expand the background and the perturbation light fields into a series of spherical harmonics. The expansion coefficients are then determined from the boundary conditions at the surface of the sphere[6]. In figure 1 the methods are compared. It shows the relative change of the fluence, that is the perturbed fluence ϕ normalized to the background fluence ϕ_0, on a line through the source and the center of the sphere. The perturbation theory agrees well with the spherical harmonics method, which indicates that it is accurate within the limits of the diffusion approximation. A meaningful comparison with the Monte Carlo simulation is prevented by the poor statistics of the result. The attempt to reduce the statistical error of the Monte Carlo simulation would lead to excessive computation time, as the accuracy increases only as the square root of the number of simulated photons. Even for this simulation the computation time was three days on a Sun SPARCstation 10. This suggests that Monte Carlo simulation is not the method of choice for this kind of geometries. The spherical harmonics expansion is considerably faster with only two minutes CPU time, but is restricted to a single spherical object. The computation time for the perturbation theory method was only 1.5 seconds. In figure 2 we demonstrate that it is capable of modeling even complex geometries in short time.

6. CONCLUSION

A perturbation theory for the steady state optical diffusion equation has been developed. The implementation in an iterative algorithm allows the modeling of light distributions in geometries with arbitrarily shaped objects within seconds. The high speed of the method suggests its use as forward algorithm in iterative imaging problems. Though the method has only been described for objects with different absorption than the background medium, it can be extended to the general case of different scattering and different absorption. In further studies we will apply the method to the time dependent diffusion equation.

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