Modeling aspects of computer analysis of light scattering from red blood cells

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Biological particles play important roles in all aspects of our life. Studying their features and behavior is of interest for a wide variety of applications, from engineering to medicine. Among other biological particles, the human red blood cell attracts special attention due to its importance for human health. In this paper modeling aspects of computer simulations of light scattering from red blood cells and some numerical methods suitable for such modeling are discussed. Recent calculation results based on an improved numerical scheme of the Discrete Sources Method are presented in comparison with results of the Discrete Dipole Approximation.

INTRODUCTION

In recent years, biological particles and their features have been studied intensively for multiple applications, from climate science to medicine. The investigation of light scattering by biological particles is considered to be an effective technique for obtaining information about their properties. This is supported by a considerable amount of modeling methods that can be applied to the theoretical study of light-scattering problems. In an ideal case the results of numerical modeling can be applied for the interpretation of measured results [1].

Human blood cells are intensively studied due to their importance for human health. Among other blood cells the Red Blood Cell (RBC, erythrocyte) attracts considerable attention due to its functions in blood and relatively simple internal structure. Biologically, the RBC is responsible for oxygen delivery over the body and change in its optical properties is a marker for certain diseases (e.g. anemia). The last fact makes its study of interest for medical diagnostic applications. In most mammals, mature RBCs lack a nucleus and organelles, typical for other cells. It makes it a convenient object for modeling methods.

MODELLING ASPECTS AND METHODS

Despite the fact the RBC has no internal structure, its complicated biconcave shape causes difficulties for modeling. In earlier works the RBC has been approached as a sphere and in some works, an equivolume sphere. Later it has been suggested to use the shape of a flat disk or oblate spheroid. Recently, it has been shown that simplified approximations that do not account for erythrocyte biconcavity in some cases deliver totally different results [2]. In the last years several shape models to approach the realistic biconcave shape have been

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suggested: Fung model, Skalak model, Lu model, Cassini-based model. Their short description is collected e.g. in [3].

In recent years different numerical methods have been applied to model the light scattering by biconcave shape models of the RBC. One of them is the Finite Difference Time Domain (FDTD) [4]. The method provides a discrete reformulation of Maxwell's equations in their differential form. It restricts the electromagnetic field problem with its open boundary problem to a simply connected and bounded space containing the region of interest. The computational domain is decomposed into a finite number of volume elements. Due to this fact the FDTD is well suitable for parallelization that helps to reduce the time of calculations. Parallelization was successfully used for calculation of RBC [4,5].

The Discrete Dipole Approximation (DDA) is another effective method for calculation of light scattering by biconcave RBCs [6]. The idea of DDA is based on a volume discretization of the investigated object. The scatterer is approximated by a lattice of dipoles, whose number depends on object shape, size, refractive index, wavelength etc. The scattering characteristics are calculated as a superposition of the dipole's fields. The main restriction of the DDA is its complexity for computation due to the growing number of dipoles used. The main challenge for DDA application consists in the low relative refractive index of RBC (1.03-1.06). The latter circumstance makes it possible to start an iterative procedure from the Born approximation, which provides reasonable values for the dipoles' polarisation. In the last years DDA has been compared to FDTD [7].

Another method suitable for modeling of biconcave RBCs is the Discrete Sources Method (DSM) [8]. The main advantage of the DSM is that it is a semi-analytical meshless method and it does not require any integration procedure. By use of this technique the scattered field everywhere outside an axially symmetric obstacle is constructed as a finite linear combination of the fields of Discrete Sources (DS) (multipoles) deposited in a complex plane adjoined to the symmetry axis of the RBC. This procedure is presented in [2] in details. The DSM solution is built to satisfy Maxwell's equations and conditions at infinity. While the most conditions of the scattering problem are satisfied analytically the unknown amplitudes of the DS are determined from transmission conditions enforced at the obstacle surface. One of the most attractive features of the DSM implementation consists in a flexible choice of the DS, which are used for the construction of the approximate solution. Besides, the DSM enables the employment of different numbers of DS used for the scattered and the internal field representation, which provides an opportunity to examine the obstacle with high refractive indices as well.

The DSM numerical scheme makes use of the axial symmetry of an obstacle's geometry and is especially suitable for biconcave shapes. Due to the multipoles' deposition in a complex plane, the DSM solution accepts the form of a finite Fourier series with respect to the azimuth angle. It allows a reduction of the surface approximation problem over the whole surface to a set of one-dimensional approximating problems enforced at the particles' meridian. To fit the transmission conditions, the generalized point-matching technique is used. It provides a considerable reduction of the sizes of linear systems and leads to a decrease of the computation time and memory storage used. The multipoles' amplitudes are determined as pseudo-solutions of over-determined systems of the linear equations. To ensure the full rank of a rectangular matrix in the over-determined system, a regularization procedure is applied.

In the last years, different shape models for RBCs have been used for light-scattering calculations based on the DSM [2,9]. The investigation of the RBC parameters on the light-scattering characteristics has been presented in [10]. The results of the DSM have been compared to results of some other numerical methods [3]. Recently it has been compared with DDA [11]. Comparison with DDA demonstrated that for RBC calculations under large scattering angles in respect to the rotational axis, DSM meets some difficulties, which are caused by a large number of Fourier harmonics needed to construct the solution. At the same time the DSM numerical scheme allows calculation of all incident angles and both polarization P and S at once, which is advantageous compared to DDA. Besides, the DSM based computer model controls convergence and stability of the results by a posterior evaluation of the surface residual at the particle surface in least-square norm [8].

NUMERICAL RESULTS

In the last months the DSM code has been improved by use of the Tikhonov's regularization in least square sense with a spectral shift in a complex plane. Due to this improvement it is now able to overcome the numerical instability observed previously.

In the following figures the results of a comparison between the DSM and DDA are presented for the element $S_{11}(\theta)$ of the Mueller Matrix [5]. For this demonstration the Fung model of the RBC [4] with a diameter D=6 µm has been taken. The wavelength is λ=496 nm (in water), the RBC refractive index is n=1.06, and the incident angle is 90°. In Fig. 1 the results based on the unmodified version of the DSM code in comparison with the results of DDA are presented (see [11]). Fig. 2 shows the same results, but for the modified DSM code. From these results it is obvious, that the modified version delivers much more stable results, which show good congruence with DDA compared to the old version.

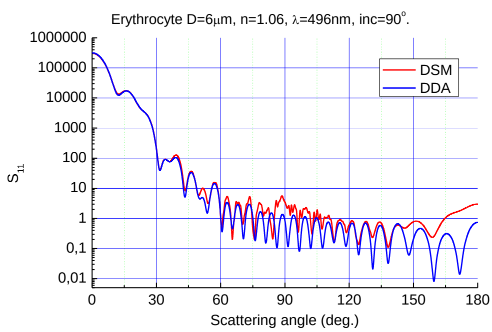

Figure 1.

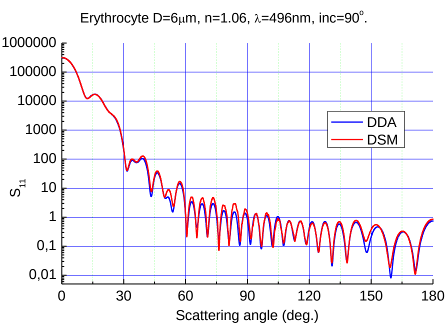

Figure 2.

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