Speckle simulator for rough surfaces using surface integral equation method and multilevel fast multiple method

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We report on a rigorous speckle simulator for three-dimensional (3D) object of general materials implemented using surface integral equation (SIE) method sped up by MLFMM. The implementation is verified by comparing the near field and far field from Ag spheres with those from Mie calculations. The capability and limitation of the simulator are further tested on spheres with different surface roughness. The simulator can calculate light scattered from objects with smooth surfaces efficiently using the MLFMM solver, and with rough surfaces using a direct LU linear equation solver.

1 Introduction

Speckle phenomena is observed normally in any coherent optical measurements. Understanding speckle field is essential for roughness evaluation, especially for inline machine processing. Thus, a physically correct modeling and simulation tool to study interactions between coherent light and rough surfaces is indispensable. For this aim, we have developed a speckle simulator using SIE method for 3D objects. Since only the surface of the object is discretized, this method shows great advantages over volumetric approaches such as the finite difference in time domain method and the frequency domain finite element method. Integral equations derived from the Maxwell's equations are usually formulated in Stratton-Chu's way. To solve the coupled electric and magnetic surface equations, we adopt the PMCHWT formulation and mesh the surface using triangular elements. Rao-Wilton-Glisson rooftops are used as basis functions [1].

To reduce memory and computation costs for large objects, an iterative solver of generalized minimal residual (GMRES) algorithm [2] sped up by multilevel fast multiple method (MLFMM) [3] was implemented. The simulator was programmed in Fortran 90 and the results for this report were calculated on a Xeon server (2× Xeon E5-2627, 3.5 GHz with 12 threads using MKL OMP algorithm).

2 Results and discussion

The speckle simulator was tested for Ag spheres with a diameter of 1 µm at the wavelength of 600 nm. The corresponding refractive index of Ag is $n = 0.0552\text{-}i4.01$ [4]. The sphere is meshed with 8584 elements having a mesh size smaller than $\lambda/10$. This results in 12876 edges and 25752 unknowns. A Gaussian random roughness with the root mean square (rms) varied from 5 nm to 35 nm and a fixed correlation length of 100 nm was generated on the sphere surface via mesh master [5].

Fig. 1(a) shows the convergence behavior for spheres with different roughness using the iterative solver GMRES combined with MLFMM. For the sphere with a smooth surface,126 iterations are needed to achieve a stop criterium, i.e., a residual error of 10^{-3}. With the increase of the roughness, the convergence is slowed down greatly. For the sphere with rms = 25 nm, 5000 iterations can only achieve an error of 2.6×10^{-2}. This is due to the fact that the condition number of the impedance matrix is increased with the surface roughness. To solve this problem, we employed a left preconditioner constituting the diagonal elements of the impedance matrix. The results using this solver are shown by the dashed lines in Fig. 1(a). The iteration number is several times reduced compared to the un-preconditioned solver. For the case with rms = 25 nm, 2632 iterations are needed.

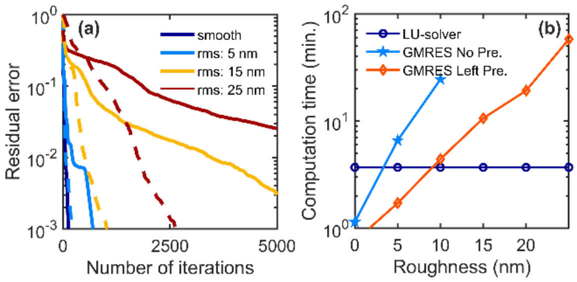

***Fig. 1** Convergence of an Ag sphere with 1 µm diameter calculated at $\lambda = 600$ nm wavelength using a GMRES solver sped up by MLFMM. Solid lines: without preconditioner; dashed lines: with a left preconditioner. (b) Time consumption of different solvers as a function of surface roughness.*

To directly compare the dependence of different solvers on the roughness, the computation costs in term of consumed time are compared in Fig. 1(b). The result from a direct equation solver using LU-decomposition (routine ZGESV in Intel MKL) is also shown, which depends solely on the number of

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unknowns. The preconditioned solver is several times faster than the un-preconditioned one. For smooth surfaces (rms = 0.0 nm), both the un-preconditioned and preconditioned solvers are much faster than the direct solver. For rms = 5 nm, the preconditioned solver is still faster than the direct solver. However, the direct solver is faster from the roughness of 10 nm on. This means, current preconditioner is not sufficient yet for surfaces with strong roughness. A more complex preconditioner such as Schur-complement preconditioner could solve the problem [6]. Nevertheless, the simulator with MLFMM can still calculate large object with smooth surfaces (e.g., 3.3 hours were consumed for smooth spheres with 0.39 million unknowns). When the number of unknows is within the limit of the computation and memory capacity, the direct solver can be employed to calculate rough surfaces as shown below.

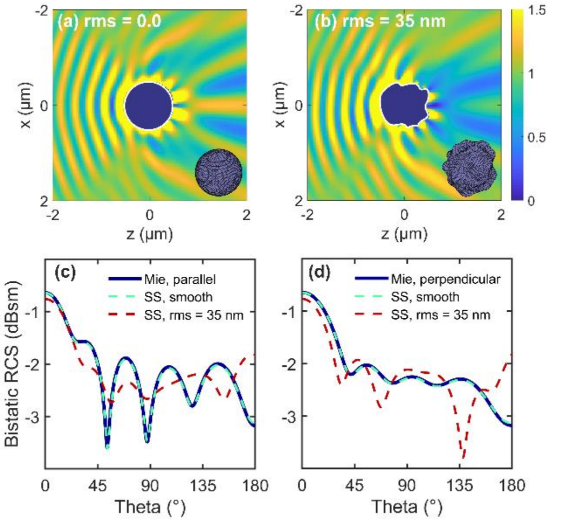

***Fig. 2** Near field intensities (including illumination) in the incident plane from (a) a smooth sphere and (b) from a sphere with a roughness of 35 nm. The spheres with meshes are shown at the lower right corner of the figures, which are illuminated by a plane wave with p-polarization (in the x-direction) propagating towards the z-direction. (c, d) Bistatic RCS in the parallel and the perpendicular plane from the two spheres shown in (a) and (b). The results are compared with the RCS results from Mie calculation (solid curves).*

Near field intensities from the spheres illuminated under a plane wave were calculated. Figs. 2(a) and (b) show the intensities in the incident *xz*-plane for the smooth sphere and the sphere with rms = 35 nm, respectively. The field in Fig. 2 (a) agrees very well with that from Mie series calculation. The near field from the sphere with roughness is distorted strongly by surface roughness as expected.

Far field bistatic radar cross section (RCS) [7] was further calculated according to

$$\sigma \sim \lim_{r\to\infty} 4\pi r^2 |E(r)|^2/|E_{in}|^2 \qquad (1)$$

Figs. 2(c) and (d) show the results in the parallel plane and perpendicular plane, respectively. The results from Mie calculation are also shown. We see that very good agreements are obtained in both planes when the surface is smooth. For the sphere with rough surface, the RCS curves are modified greatly, the information of which can be used to evaluate surface roughness and we will report this in reports.

3 Conclusion

We have developed a rigorous speckle simulator using SIE for 3D object. The simulator can solve linear matrix vector equation using the direct LU-solver or an iterative solver (GMRES) sped up by MLFMM. For objects with smooth surfaces, the latter solver is efficient in both computation and memory cost. Once the surface becomes rough, current preconditioner for the iterative solver is insufficient. More complex preconditioner could solve the problem.

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