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Extension of the program 3D MMP with a fifth order Gaussian beam

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Indexing terms: Electromagnetic wave scattering, Modelling

The authors have extended Hafner and Bomholt's numerical electromagnetic scattering program 3D MMP [1] with a fifth order Gaussian beam approximation using Barton and Alexander's equations from [2]. Numerical computation results for one spherical particle located on-axis in a highly focussed Gaussian beam ($s = 0.1$) serve as an example for high accuracy scattering simulations in the visual spectral range at low size parameters ($\alpha = 20$).

Introduction: A good mathematical description of a Gaussian laser beam has been known since Davis' first order approximation [3]. Owing to a boost in computing power in the 1980s, different numerical methods for electromagnetic scattering computations had been developed. In addition, former scattering theories had to be modified to integrate the Gaussian beam description as well. In most cases this task is solved by expanding the Gaussian beam as a spectrum of plane waves or as spherical vector wave functions. Extensions like these are usually quite complicated and time consuming to realise. Also, these methods often lack accuracy for non-spherical and off-beam axis pafticle systems. Numerical calculation of highly focused laser beams of $s \gtrsim 0.07$ ($s = 1/k\omega_0$; k is the wave number, ω_0 is the beam waist radius) demand a higher accuracy than the common Davis first order approximation.

Theoretical background: The versatile multiple multipole (MMP) method was originally developed for numerical simulations of 3-D electromagnetic scattering problems in the HF region. The scattering media, which have to be isotropic and homogeneous, are divided into domains of constant optical properties. The total electromagnetic field is divided into a known incident and the unknown scattered and induced (internal) fields. The unknown fields, which have to fulfill the 3-D Helmholtz equations, are approximated by sets of multipoles with different origins. The arbitrary, analytically known field function of the excitation only has to contain its numerical field values at the boundary. Therefore, we could use the solution Barton and Alexander derived for a fifth order description for all six electromagnetic field components. The equations are power series of the parameter s (for exact equations see [2]). The accuracy of the Gaussian beam description depends on the parameter s, since the exponent of s characterises the order of approximation. According to [2], the first order is accurate to $s \leq 0.07$, and the fifth order is accurate to $s \leq 0.20$, if the maximum percent error of the solution to Maxwell's equations should not exceed 1.2%.

Computation results: We generated a Fortran 77 code for the equations and implemented it in 3D MMP. To check the new code, we carried out various scattering computations. In this paper we mainly concentrate on the Gaussian beam effects, therefore we only present results for one spherical particle in vacuum, with its centre positioned at the focal point and a beam parameter of $s = 0.1061$ ($\omega_0 = 1.5\lambda$). For further calculation parameters see subcaptions of the figures. Fig. 1 shows three far-field scattering curves; the scattering angle was scanned perpendicular relative to the scattering plane. The curves are calculated with the first and fifth order MMP, and the localised approximation [4] for verification. We then took the fifth order as a reference and plotted the absolute intensity differences to its lower orders (Fig. 2, showing two curves). Scattered power is distributed over six magnitudes. As can be seen, the higher orders result in more detail in the scattered field. The largest absolute deviations (errors) to the fifth order do not occur in the backscattering region but predominatly in the forward direction. The localised approximation is roughly equivalent to the fifth order of Barton *et al.*.

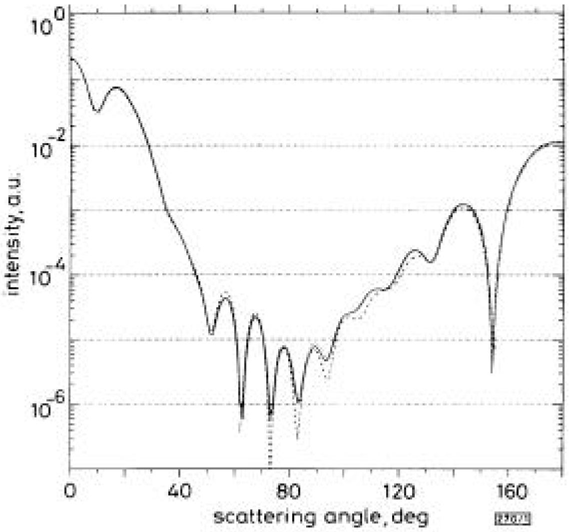

Fig. 1 *Far-field scattering diagram*

——— fifth order
– – – – first order
·········· localised approximation

TM polarisation (electric field vector is perpendicular to scattering plane), particle radius $r = 0.5\mu m$, refractive index $n = 1.334$, size parameter $\alpha = 2\pi r/\lambda = 20.0$ (λ: wavelength of the Gaussian laser beam)

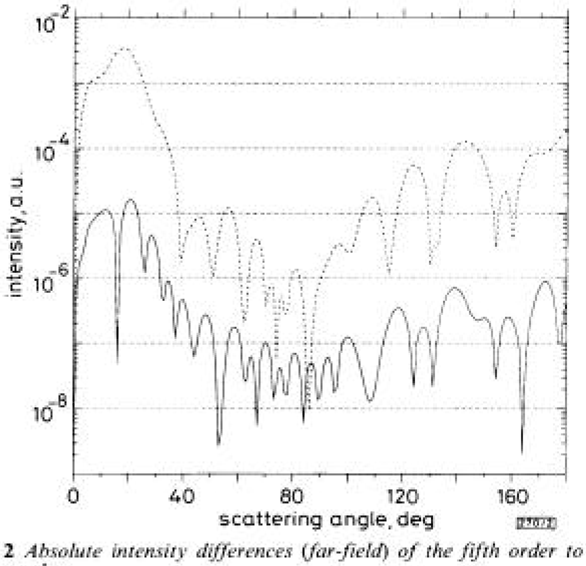

Fig. 2 *Absolute intensity differences (far-field) of the fifth order to its lower orders*

——— fourth order
– –.– – third order

Conclusion: The first order should be a sufficient approximation for most cases. We conclude that higher approximations than the second, or even third order are only neccessary for very tightly focused beams or off-beam axis particles. Approximations better than the fifth order do not make sense due to negligible gain in accuracy and strucure. In addition, the limit of physical beam propagation is about to be reached when $\omega_0 \rightarrow \lambda$ (and therefore $s \rightarrow 0.159$). 3D MMP can be used for scattering computations of non-spherical particles, as well as for multiple scattering. Since we have extended this method to Gaussian beam scattering, it is possible to simulate laser measurements in the range of homogeneous particles in general. Limits of application depend on the efficiency of the source code and hardware.

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