Towards efficient modelling of optical micromanipulation of complex structures

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Abstract

Computational methods for electromagnetic and light scattering can be used for the calculation of optical forces and torques. Since typical particles that are optically trapped or manipulated are on the order of the wavelength in size, approximate methods such as geometric optics or Rayleigh scattering are inapplicable, and solution or either the Maxwell equations or the vector Helmholtz equation must be resorted to. Traditionally, such solutions were only feasible for the simplest geometries; modern computational power enable the rapid solution of more general—but still simple—geometries such as axisymmetric, homogeneous, and isotropic scatterers. However, optically-driven micromachines necessarily require more complex geometries, and their computational modelling thus remains in the realm of challenging computational problems. We review our progress towards efficient computational modelling of optical tweezers and micromanipulation, including the trapping and manipulation of complex structures such as optical micromachines. In particular, we consider the exploitation of symmetry in the modelling of such devices.

1 Introduction

Optical tweezers have seen deployment in a wide range of applications in biology, soft materials, microassembly, and other fields. As well as being used for the trapping and manipulation of a wide range of natural and artificial objects, optically trapped probes are used to measure forces on the order of piconewtons. Compared with this diverse range of experimental applications, theory and accurate computational modelling of optical tweezers has received much less attention and has remained relatively undeveloped, especially for non-spherical particles and non-Gaussian beams. This is unfortunate, especially when we consider the growing fields of controlled rotation of complex microparticles—prototype optically-driven micromachines—and fully three-dimensional manipulation using complex optical fields, where the application of theory and modelling provide insight into the physics, and allow engineering and optimisation.

Since optical forces and torques result from the transfer of momentum and angular momentum from the trapping beam to the particle via scattering, the theory and computational modelling of optical tweezers is, in essence, the theory and computational modelling of the scattering of light or electromagnetic radiation. Since typical particles that are optically trapped or manipulated are on the order of the wavelength in size, approximate methods such as geometric optics or Rayleigh scattering are inapplicable, and solution or either the Maxwell equations or the vector Helmholtz equation must be resorted to. As scattering by particles in this size range is of interest in many fields, a wide variety of analytical and computational methods have been developed. Thus, there is a solid foundation on which to develop computational modelling of optical micromanipulation.

There are, however, complications that prevent simple direct application of typical light-scattering codes. The first, but not necessarily the most important, is that optical tweezers makes use of a highly focussed laser beam, while most existing scattering codes assume plane wave illumination. Perhaps more fundamental is the need for a large number of repeated calculations to characterise an optical trap—even for an axisymmetric (but nonspherical) particle trapped in a circularly polarised Gaussian beam, we already have four degrees of freedom. Clearly, this places strong demands on computational efficiency.

Due to this requirement for repeated calculation of scattering by the same particle, we employ the T-matrix method [1, 2]. Below, we outline the employment of the T-matrix method for the calculation of optical forces and torques. While most implementations of the T-matrix method are restricted to simple geometries, this is not a limitation inherent in the method; fundamentally, the T-matrix method is a *description* of the scattering properties of a particle, not a method of calculating the scattering properties. Therefore, in principle, any method of calculating scattering can be used to obtain the T-matrix for a scatterer. We discuss such "hybrid" methods, where a computational method not usually associated with the T-matrix method is used to calculate the T-matrix of a scatterer, and hence the optical force and torque.

A further important consideration is that optical micromachines, while complex, are likely to possess a high degree of symmetry; this can be exploited to reduce computation times by orders of magnitude. We demonstrate the effectiveness of this approach by modelling the optical trapping and rotation of a cube. The two principal symmetries of such shapes—mirror symmetry and discrete rotational symmetry about the normal to the mirror symmetry plane—are exactly the symmetries that typify the ideal optically-driven rotor.

2 *T*-matrix formalism for optical force and torque

The *T*-matrix method in wave scattering involves writing the relationship between the wave incident upon a scatterer, expanded in terms of a sufficiently complete basis set of functions $\psi_n^{(\text{inc})}$, where n is a mode index labelling the functions, each of which is a solution of the Helmholtz equation,

$$U_{\text{inc}} = \sum_n^\infty a_n \psi_n^{(\text{inc})}, \tag{1}$$

where a_n are the expansion coefficients for the incident wave, and the scattered wave, also expanded in terms of a basis set $\psi_k^{(\text{scat})}$,

$$U_{\text{scat}} = \sum_k^\infty p_k \psi_k^{(\text{scat})}, \tag{2}$$

where p_k are the expansion coefficients for the scattered wave, is written as a simple matrix equation

$$p_k = \sum_n^\infty T_{kn} a_n \tag{3}$$

or, in more concise notation,

$$\mathbf{P} = \mathbf{TA} \tag{4}$$

where T_{kn} are the elements of the *T*-matrix. The *T*-matrix formalism is a Hilbert basis description of scattering. The *T*-matrix depends only on the properties of the particle—its composition, size, shape, and orientation—and the wavelength, and is otherwise independent of the incident field.

This means that for any particular particle, the *T*-matrix only needs to be calculated once, and can then be used for repeated calculations. This is the key point that makes this an attractive method for modelling optical tweezers, providing a significant advantage over many other methods of calculating scattering where the entire calculation needs to be repeated.

The natural choice of basis functions when describing scattering by a compact particle is to use vector spherical wavefunctions (VSWFs) [1]. The optical force and torque are given by sums of products of the modal amplitudes [3, 4, 5].

Notably, neither how the VSWF expansion of the incident field nor how the *T*-matrix can be calculated has entered the above description of scattering. A variety of methods exist for the former [6, 5], and the latter task is generally the more challenging computationally.

Most implementations of the *T*-matrix method use the extended boundary condition method (EBCM), also called the null field method, to calculate the *T*-matrix. This is so widespread that the *T*-matrix method and the EBCM are sometimes considered to be inseparable, and the terms are sometimes used interchangeably. However, from the description above, it is clear that the *T*-matrix formalism is independent of the actual method used to calculate the *T*-matrix [7, 8].

A number of alternative methods have been used for the calculation of *T*-matrices. Notably, such "hybrid" methods, for example the discrete dipole approximation (DDA) method used by Mackowski [9] can be used for the calculation of *T*-matrices for particles of arbitrary shape, internal structure, and electromagnetic properties. Complex internal structure will generally require a discretisation of the internal volume of the particle, rather than a method based on surface discretisation. We are working on both finite-difference frequency-domain (FDFD) and DDA based hybrid *T*-matrix solvers.

3 Optical torque and symmetry

The *T*-matrix elements are strongly dependent on the symmetry of the scatterer [1]. We can deduce the principal features from Floquet's theorem, relating solutions to differential equations to the periodicity of their boundary conditions.

If we have a scatterer with nth-order rotational symmetry about the z-axis, an incident mode of azimuthal index m couples to scattered modes with azimuthal indices $m, m \pm n, m \pm 2n, m \pm 3n$ and so on. For scatterers

that are mirror-symmetric, upward and downward coupling must be equal, in the sense that, for example, a mirror-symmetric scatterer of 2nd order rotational symmetry (such as a long rod), T-matrix elements coupling from $m = 1$ modes to $m = -1$ modes will have the same magnitudes as the elements coupling from $m = -1$ to $m = 1$ modes. For chiral scatterers, these T-matrix elements will, in general, be different.

This directly affects the optical torque; the vector spherical wavefunctions are eigenfunctions of the angular momentum operators J^2 and J_z. Essentially, the radial mode index n gives the magnitude of the angular momentum flux, while the azimuthal mode index m gives the z-component of the angular momentum flux. Therefore, the coupling between orders of different m describes the generation of optical torques about the beam axis.

For the case of a rotationally symmetric scatterer, this means that there is no coupling between modes with differing angular momenta about the z-axis[1, 10, 11]. Therefore, it is not possible to exert optical torque on such scatterers except by absorption (or gain)—since the incoming and outgoing angular momenta per photon are the same, the only optical torque can result from a change in the number of photons. In general, the use of absorption for the transfer of optical torque is impractical, due to excessive heating. Therefore, a departure from rotational symmetry is required. This can be either at the macroscopic (the shape of the particle) or microscopic (optical properties of the particle) level.

Birefringent and elongated or flattened particles are simple examples of introducing such asymmetry; notably, such particles were the first to be controllably optically rotated through means other than absorption, for example by Beth in the first measurements of optical torque [12]. Particles with these properties have also been rotated in optical traps [13, 14, 15, 16]. As such particles can still be axisymmetric about one axis, rapid calculation of optical forces and torques is still possible [15, 16]

More complex particles have also been fabricated and rotated [17, 18, 19], but in these cases, there are few results from computational modelling [20].

As such structures typically possess discrete rotational symmetry, the restrictions on coupling between azimuthal orders can be used to reduce the number of T-matrix elements that need to be calculated. This can greatly reduce the time required. This is also the case for the hybrid methods described above. For a scatterer with pth-order discrete rotational symmetry, it is only necessary to perform calculations for a $1/p$ portion of the entire structure. If, in addition, there is mirror symmetry about the xy plane, the parity of the VSWFs will be preserved. Therefore, an odd-n TE mode will only couple to odd-n TE modes and even-n TM modes. This halves number of non-zero T-matrix elements, and halves the portion of the structure that needs to be modelled.

4 Example: optical trapping of a cube

A simple example illustrating both the relationship between optical torque and symmetry, and the exploitation of particle symmetry for more efficient calculation of optical forces and torques, is the optical trapping of a cube. The cube embodies both of the symmetries—mirror symmetry and discrete rotational symmetry about the normal to the mirror symmetry plane—that typify the ideal optically-driven rotor.

As the cube has 4th-order rotational symmetry, and mirror symmetry with respect to the Cy plane, each incident modes only couples to approximately $1/8$ the number of significant scattered modes. Although the column-by-column calculation of the T-matrix still requires the same number of least-squared solutions, each of this is of a smaller system of equations, and much faster. For example, the two wavelengths wide cube used in our example below required 30 minutes for the calculation of the T-matrix on a 32 bit single-processor 3 GHz microcomputer, as compared with 30 hours for an object of the same size lacking the cube's symmetries. Only one octant of the cube was explicitly included in the calculation.

If figure 1, we show the optical force and torque exerted on a cube with relative refractive index of $1.19 = 1.59/1.34$, and faces 2λ across, where λ is the wavelength in the surrounding medium. Once the T-matrix is calculated, to calculate the optical force and torque at a particular position requires less than 1 second (unless the point is far from the beam focus, in which case, up to 10 seconds or so can be needed).

In figure 1(a), we see that cubic shapes can be stably trapped axially, while 1(b)–(d) show that optical torque can be generated by such structures. The increased efficiency resulting from the use of orbital angular momentum [5] is clear.

5 Conclusion

The symmetry properties of a scatterer can be used to dramatically speed the calculation of the scattering properties of a particle. If these are expressed in the form of the T-matrix, this enables rapid and efficient calculation of optical forces and torques. Since typical optically-driven microrotors possess discrete rotational symmetry, they are ideal candidates for this method. In addition, mirror symmetry about a plane can also
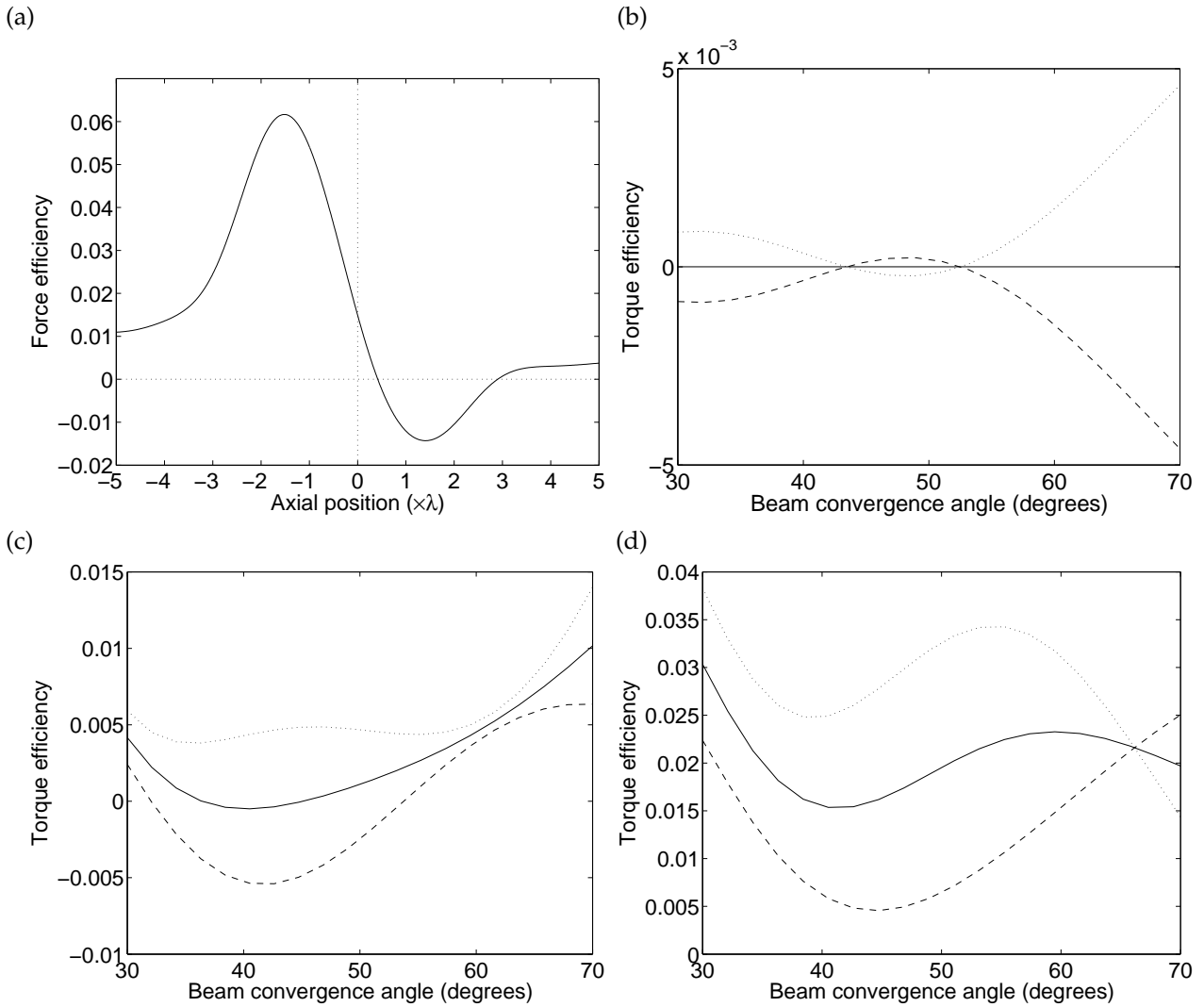
Figure 1: Optical force and torque on a dielectric cube. (a) shows the axial force as a function of position along the beam axis, showing that the cube can be trapped. (b)–(d) show the dependence of the optical torque on the beam convergence angle and the polarisation and orbital angular momentum. In (b), the beam is Gaussian (ie LG_{00}), while in (c) and (d), the beams are LG_{01} and LG_{02} respectively. The solid lines are for plane polarised beams, while dotted and dashed lines are for circularly polarised beams with spin parallel to and antiparallel to the orbital angular momentum.

be used to further reduce the computational burden. Finally, "hybrid" T-matrix methods can be used for particles with geometries or internal structure making them unsuitable for traditional methods of calculating T-matrices.

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