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Fast and accurate algorithm for repeated optical trapping simulations on arbitrarily shaped particles based on boundary element method

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ABSTRACT

In optical trapping applications, the optical force should be investigated within a wide range of parameter space in terms of beam configuration to reach the desirable performance. A simple but reliable way of conducting the related investigation is to evaluate optical forces corresponding to all possible beam configurations. Although the optical force exerted on arbitrarily shaped particles can be well predicted by boundary element method (BEM), such investigation is time costing because it involves many repetitions of expensive computation, where the forces are calculated from the equivalent surface currents. An algorithm is proposed to alleviate the difficulty by exploiting our previously developed skeletonization framework. The proposed algorithm succeeds in reducing the number of repetitions. Since the number of skeleton beams is always much less than that of beams in question, the computation can be very efficient. The proposed algorithm is accurate because the skeletonization is accuracy controllable.

1. Introduction

The manipulation of micro-/nano-particles based on the optical forces [1–3] offers many benefits over its competing technologies, most notably the ability to work with delicate or potentially harmful samples in sealed environments without direct mechanical access. In order to achieve a deep understanding and thus an optimized optical trapping, it is important to predict the radiation pressure force (RPF) exerted on the micro-/nano-particles.

There are many well-developed methods to predict RPF suitable for different scenarios as the behavior of optical trapping depends upon the size of the trapped particle relative to the working wavelength of the light. If the particle dimensions are much smaller than the wavelength of light, the particles can be treated as electric dipoles in the electric field. In cases where the dimensions of the particle are much greater than the wavelength, a simple ray optics treatment is sufficient. When the objects are of dimensions within the resonance region, e.g., an order of magnitude of the trapping beam wavelength, the only accurate models involve the treatment of either time dependent or time harmonic Maxwell's equations using appropriate boundary conditions. These models can be generally grouped into analytical approaches or full-wave algorithms. Analytical methods are always limited to particles with canonical shapes while full-wave ones are always expensive. In [4–7], analytical algorithms focused on the spherical particles have been reported. It is a much more difficult task to predict the RPF exerted on nonspherical particles. Many efforts have been reported on this topic [8–14].

It has been shown that boundary element method (BEM) solutions of surface integral equations (SIEs), named after method of moments (MoM) in many studies, are among the most popular ones [15], due to their versatility and accuracy. Most recently, multilevel fast multipole algorithm (MLFMA), one of the most widely used full-wave method in computational electromagnetic community, has been employed to accelerate the BEM solution for the prediction of RPF exerted on arbitrarily shaped particles [16].

It is well-known that the optical force depends not only on the property of the target itself but also on the configuration of the incident beam [17–19]. For example, the force exerted by Gaussian beams varies much with the position of the beam center as well as the beam waist [16,20]. In another word, to reach desired performance of trapping, it is important to optimize the configuration of the incident beam. Additionally, several quantities should be studied to describe the most important properties of the optical trap, including the trap strength, equilibrium position and spring constant [21]. A large number of repeated computations for a same particle are unavoidable for achieving sufficient spatial resolutions of these quantities. A simple but reliable manner in realizing such investigation is to compute the RPFs within the parameter space point by point. However, the associated study in terms of BEM can

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be a critical issue because it would degrade the efficiency of the simulation significantly. BEM often employs the intermediate parameter as unknown, e.g., the equivalent surface current. After obtaining the equivalent currents for a given beam, we should compute the required RPF from the currents. In [22,23], several approaches to computing the optical force were compared in terms of accuracy and efficiency. The most efficient manner is to calculate the force directly from the currents on the scatterer surface, which takes $O(n)$ time only. However, the approach would lead to inaccurate RPF evaluation for some cases [23]. The approach based on Maxwell's tensor is immune from this problem but is less efficient. The cost reaches as high as $O(np)$ with n and p the number of unknowns and sampling points. In general, p is comparable to n for an accurate evaluation of RPF, giving rise to the complexity of $O(n^2)$. For the sake of generality, the approach based on Maxwell's tensor is employed in this work. Consequently, the cost of computing optical forces from equivalent currents is $O(mn^2)$ for the case with m beams or repetitions. To make it worse, m is huge in many applications because the investigation often relates with serval parameters, each ranging in a wide span. For example, it requires at least 7 parameters to completely describe a Gaussian beam, including the beam center (x_o, y_o, z_o), the beam waist w_o, the beam propagating direction (θ_o, ϕ_o), and the beam polarization. The total number of beams produced is $m = m_o^6$, where we assume that the number of samplings for each parameter is identical and denoted by m_o.

The translation of equivalent currents to the RPFs becomes a bottleneck for the simulation. We propose a novel algorithm to alleviate the difficulty by reducing the number of repetitions. The proposed approach is based on the concept of skeleton [24–29]. In [20], the skeletonization technique has been exploited to accelerate the BEM solution. Generally, skeletonization is equivalent to finding principal elements, e.g., light beams in [20]. The incident beams can be viewed as elemental excitations, which can be ranked in terms of their contributions to the performance of the optical system. This amounts to generating an ordering of all beams [20]. Different from [20], where efforts have been put on how to select skeleton efficiently, we focus on reducing the repetitions related to translating equivalent currents to RPFs in this work. Because the skeletonization is accuracy controllable, the accuracy of the proposed scheme is well-controlled. Since the number of skeleton beams is generally much less than the total number of beams, the acceleration rate can be high. Although the proposed scheme is discussed and validated in terms of BEM, it can be easily extended to other methods. It should be noted that the present algorithm is incapable of angular sweeping. How to address the difficulty is our future work.

The remainder of the paper is organized as follows. Section 2 discusses the theoretical and technical background. Section 3 details the proposed algorithm. Section 4 gives the simulation results to show performance of the proposed algorithm. Section 5 concludes the paper.

2. Theoretical and technical background

In this section, we introduce the technique background of the proposed method, including the BEM discretization of SIE, the skeletonized system with many incident beams and the approach to compute RPF.

2.1. Surface integral equations and boundary element method

Suppose the arbitrarily shaped homogeneous particle is embedded in an homogeneous medium, upon the incident light ($\mathbf{e}^{\mathrm{inc}}$, $\mathbf{h}^{\mathrm{inc}}$), the scattered fields ($\mathbf{e}^{\mathrm{sca}}$, $\mathbf{h}^{\mathrm{sca}}$) at observation $\mathbf{r}$ can be expressed in SIEs by the form of [30]

$$\mathbf{e}_{\mathrm{i/e}}^{\mathrm{sca}}(\mathbf{r}, \mathbf{j}_{\mathrm{i/e}}, \mathbf{m}_{\mathrm{i/e}}) = \eta_{\mathrm{i/e}} \mathcal{L}_{\mathrm{i/e}}(\mathbf{j}_{\mathrm{i/e}}) - \mathcal{K}_{\mathrm{i/e}}(\mathbf{m}_{\mathrm{i/e}}), \tag{1a}$$

$$\mathbf{h}_{\mathrm{i/e}}^{\mathrm{sca}}(\mathbf{r}, \mathbf{j}_{\mathrm{i/e}}, \mathbf{m}_{\mathrm{i/e}}) = \eta_{\mathrm{i/e}}^{-1} \mathcal{L}_{\mathrm{i/e}}(\mathbf{m}_{\mathrm{i/e}}) + \mathcal{K}_{\mathrm{i/e}}(\mathbf{j}_{\mathrm{i/e}}), \tag{1b}$$

where $(\mathbf{j}_{\mathrm{i/e}}, \mathbf{m}_{\mathrm{i/e}})$ are the equivalent electric and magnetic currents. The subscript "i" denotes the interior region of the target/particle V and "e" stands for the exterior region. $\eta_{\mathrm{q}} = \sqrt{\mu_{\mathrm{q}}/\epsilon_{\mathrm{q}}}$, (q = i/e) is the the wave impedance for region q with ϵ_{q} the permittivity and μ_{q} the permeability. In above expressions, the time factor $e^{-j\omega t}$ of the angular frequency ω is dropped for conciseness.

The operators $\mathcal{L}$ and $\mathcal{K}$ corresponding to the region q can be written as

$$\mathcal{L}_q\{\mathbf{X}\}(\mathbf{r}) = -jk_q \int_S dS' \left[\mathbf{I} + \frac{1}{k_q^2}\nabla\nabla'\cdot\right]\mathbf{X}(\mathbf{r}')g_q(\mathbf{r}, \mathbf{r}'), \tag{2a}$$

$$\mathcal{K}_q\{\mathbf{X}\}(\mathbf{r}) = -\frac{\Omega(\mathbf{r})}{4\pi}\mathbf{X}(\mathbf{r}') + \nabla \times \fint_S dS' g_q(\mathbf{r}, \mathbf{r}')\mathbf{X}(\mathbf{r}'), \tag{2b}$$

where $\fint$ stands for the principal value integration; $0 \le \Omega(\mathbf{r}) \le 4\pi$ is the internal solid angle; $g_q(\mathbf{r}, \mathbf{r}') = \frac{e^{-jk_q|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$, denotes the homogeneous-space Green's function with $k_q = \omega\sqrt{\mu_q\epsilon_q}$ the wavenumber for the region q.

The surface currents $(\mathbf{j}_{\mathrm{q}}, \mathbf{m}_{\mathrm{q}})$ are defined as

$$\mathbf{j}_{\mathrm{q}} = \hat{n}_{\mathrm{q}} \times \mathbf{h}_{\mathrm{q}}^{\mathrm{tot}} \quad \text{and} \quad \mathbf{m}_{\mathrm{q}} = \mathbf{e}_{\mathrm{q}}^{\mathrm{tot}} \times \hat{n}_{\mathrm{q}} (\mathrm{q} = \mathrm{i/e}), \tag{3}$$

where $\hat{n}_{\mathrm{i/e}}$ is the inward/outward unit vector normal to the closed surface S bounding V. More precisely, $\hat{n}_{\mathrm{e}} = -\hat{n}_{\mathrm{i}}$. The total electric and magnetic fields $\mathbf{e}_{\mathrm{q}}^{\mathrm{tot}}$ and $\mathbf{h}_{\mathrm{q}}^{\mathrm{tot}}$ are in the form of

$$\mathbf{e}_{\mathrm{q}}^{\mathrm{tot}}(\mathbf{r}) = \mathbf{e}_{\mathrm{q}}^{\mathrm{sca}}(\mathbf{r}, \mathbf{j}_{\mathrm{q}}, \mathbf{m}_{\mathrm{q}}) + \mathbf{e}^{\mathrm{inc}}, \tag{4a}$$

$$\mathbf{h}_{\mathrm{q}}^{\mathrm{tot}}(\mathbf{r}) = \mathbf{h}_{\mathrm{q}}^{\mathrm{sca}}(\mathbf{r}, \mathbf{j}_{\mathrm{q}}, \mathbf{m}_{\mathrm{q}}) + \mathbf{h}^{\mathrm{inc}}. \tag{4b}$$

Distinct SIE formulations can be obtained by combining differently scaled tangential and/or normal forms of Eq. (4) along with the boundary condition $\mathbf{j} = \mathbf{j}_{\mathrm{e}} = -\mathbf{j}_{\mathrm{i}}$ and $\mathbf{m} = \mathbf{m}_{\mathrm{e}} = -\mathbf{m}_{\mathrm{i}}$ [31]. In this work, the SIE of the combined tangential field (CTF) formulation [31] is employed for the computation on dielectric targets. Meanwhile, for the computation on metallic nanostructures, we utilize the SIE of the PMCHW (Poggio, Miller, Chang, Harrington, Wu) formulation for high accuracy.

With the standard BEM procedure and Rao-Wilton-Glisson (RWG) functions [30,31,16,22,32], the SIE can be recast into the matrix form as

$$\begin{bmatrix} \mathbf{Z}^{\mathrm{J,J}} & \mathbf{Z}^{\mathrm{J,M}} \\ \mathbf{Z}^{\mathrm{M,J}} & \mathbf{Z}^{\mathrm{M,M}} \end{bmatrix} \cdot \begin{bmatrix} \mathbf{x}^{\mathrm{J}} \\ \mathbf{x}^{\mathrm{M}} \end{bmatrix} = \begin{bmatrix} \mathbf{b}^{\mathrm{J}} \\ \mathbf{b}^{\mathrm{M}} \end{bmatrix}, \quad \text{or} \quad \mathbf{Z}\cdot\mathbf{x} = \mathbf{b}, \tag{5}$$

where $\mathbf{Z}$ is the impedance matrix; $\mathbf{x}$ is the coefficient vector representing $(\mathbf{j}, \mathbf{m})$ and $\mathbf{b}$ is the vector related with the incident light beam $(\mathbf{e}^{\mathrm{inc}}, \mathbf{h}^{\mathrm{inc}})$. Generally, for targets large in size, iterative solver in combination with some fast algorithm, such as MLFMA [33,34], should be employed to accelerate the solution of Eq. (5). We use our well-developed MLFMA [35,36] for the acceleration.

2.2. System with many incident beams and skeletonization

As we are interested the system with many incident beams, it is convenient to extend the vectors $\mathbf{b}$ and $\mathbf{x}$ to matrices, denoted by $\mathbf{B}$ and $\mathbf{X}$, respectively. The associated matrix system can thus be

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