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Calculating optical forces using the boundary integral method

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Abstract
In this paper, we show that the boundary integral method is highly efficient for the calculation of optical forces on small dielectric and metallic objects. The boundary integral formulation for the Maxwell equations is stated, and an implementation of the equations is described, tested and used to derive new bistability results for two dielectric spheres in counterpropagating incoherent laser beams.

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1. Introduction

A large class of computational problems in optics, and photonics in particular, involves the scattering of light by linear materials that have piecewise constant material constants. In many cases, the light sources are approximately monochromatic. It is furthermore typically the case in which the values of the electric and magnetic field components are only needed in a limited part of what is usually a noncompact domain. This is particularly true for near-field optics and for the calculation of resonances and optically induced forces. Under these circumstances, domain-based methods like the finite difference time domain method (FDTD) [18, 19, 21], finite element methods [2, 9, 20] or Galerkin methods in general have major shortcomings with respect to efficiency, numerical stability and implementational complexity. The basic source of the weaknesses is the presence of noncompact domains and discontinuous coefficients in the Maxwell equations. Both issues can be, and have been, addressed and methods have been developed that to some extent solve the problems. The noncompact domain problem has been addressed by the development of the perfectly matched layer (PML) [3, 8] where the computational domain is surrounded on all sides by a layer that perfectly absorbs all waves and thus in theory gives a perfect simulation of a noncompact domain. In practice, a certain amount of tuning is however necessary to balance the level of reflection against the computational resources that are to be allocated to the computation inside the layer. If this is not optimized carefully, one can easily end up using a large fraction of the computational resources in the PML layer. The presence of the layer certainly introduces complexities in the implementation and purely mathematical issues that are not part of the actual physical model. The problems stemming from the discontinuous coefficients have been addressed by introducing nonuniform computational grids and by the smoothing of the discontinuous domain boundaries. In many situations, this takes care of the worst problems but at, in many cases, a significant additional complexity in the implementation and computational stability and cost. Even if we assume that the domain methods are perfected and that problems like the ones discussed here are fully solved, we are still left with the fact that the domain methods compute the fields at all points of the domain, whereas the values are in many cases only needed in a small part of the domain. This is an irreducible problem for any domain-based method.

It is well known in other areas of computational physics, but may not be so well known in computational photonics, that for the type of computational problem described in this paper, the method of choice is the boundary integral method (BIM). In this method, the governing differential equations are reformulated as integral equations involving unknown fields only on the surfaces separating the domains defined by constant material parameters. Since these surfaces typically are compact whereas the whole domain is noncompact, we have effectively removed one whole space dimension from the problem. The fields at any particular point in the domain can be computed from the field values on the bounding surfaces by using certain integral identities. These calculations come of course at an additional computational cost, beyond the one required for the solution of the integral equations, and if the values of the fields at all points in a large domain are needed, the cost can be prohibitive. However, in few, if any, experimental situations are the fields in large domains measured, or even of interest. Usually, the parameters measured are collective parameters that can be calculated from the surface values of the fields at low computational cost. A typical example of this is the computation of optically induced forces. We are aware of the fact that there are still unresolved issues surrounding the calculation of such forces and even their precise definition [5, 11]. We will here assume that the forces can be calculated by using a stress tensor. Usually for optical applications, we use the Minkowski stress tensor but the point we are making here is in no way dependent on the choice of this particular tensor. Calculation of the force using the Minkowski stress tensor requires the values of all the fields on the bounding surface defining the object and only these values. In this sense, the BIM is optimal for computing optical forces; one can compute exactly what is needed and no more. The calculation of resonance curves can also be reduced to a calculation involving the surface fields only and the BIM is thus optimal for such calculation also.

The BIM is not however without problems of its own. The two foremost are related to the singular behavior of Green's functions when the source point and the observation point coincide and to the fact that, in many cases, discretization leads to nonsparse nonsymmetric matrices whose matrix elements are difficult to compute. The first problem becomes more severe as the dimensionality of the problem increases and is particularly severe for three-dimensional (3D) electromagnetic scattering from dielectric and nonideal conductors. The BIM equations for this case cannot be said to be directly derived from the Maxwell equations but are rather consistent with the Maxwell equations and a natural regularization procedure. The BIM equations for the electromagnetic case are usually called the Müller scattering equations [14, 15, 17], but we are aware of the fact that there are other boundary integral formulations of the Maxwell equations known in the research literature [6]. The regularization procedure does not remove the singularity from the BIM equation, but only makes it integrable. The issue of how to handle the resulting 2D principal value integral numerically is of central concern and will be addressed in detail. The nonsymmetry and nonsparsity of the matrices resulting from the discretization can not be evaded and must be faced head on. The nonsymmetry, nonsparseness and high computational cost of computing the matrices resulting from any discretization of the BIM has traditionally been considered as a major drawback, even a fatal one. There used to be a certain amount of truth in this criticism, but with the shift in computational platforms from serial to large scale parallel clusters, this criticism has lost much of its force. In fact, in a highly parallel computational environment, it is desirable to shift the computational work from the solution of linear systems to the computation of the matrix for the system. This is because the computation of the matrix elements is trivially 100% parallelizable whereas the solution of the linear systems is not. Thus in the current computational environment, it is actually preferable to shift the workload from solving linear systems to computing the matrix for the linear system and this is exactly what the BIM achieves.

The paper is organized in the following way. In section 2, we formulate the Müller scattering equations for multiple scattering objects. Issues relating to the discretization, numerical implementation and efficiency are discussed in section 3. This section also contains a detailed comparison of the exact Mie solution [4, 13] for single spheres and for two concentric spheres [1]. We discuss both surface field values and optical forces. The problem of optically induced forces between dielectric spheres in counterpropagating incoherent Gaussian beams has been discussed both experimentally and numerically using the paraxial beam propagating method [12] and the coupled dipole method [10]. In section 4, optical forces are computed for the two-sphere system using the BIM. Section 5 contains a summary. The Müller scattering equations are derived in the appendix.

2. The Müller scattering equations

The basic mathematical model describing the type of systems discussed in the introduction are the frequency domain Maxwell equations for linear nonmagnetic dispersive materials:

$$\begin{aligned} \nabla\times\mathbf{E}-\mathrm{i}\omega\mathbf{B}&=0,\\ \nabla\times\mathbf{B}+\mathrm{i}\omega\varepsilon_0\mu_0 n^2\mathbf{E}&=\mathbf{j},\\ \nabla\cdot\mathbf{B}&=0,\\ \nabla\cdot(\varepsilon_0 n^2\mathbf{E})&=\rho. \end{aligned}$$

The charge density ρ and the current density $\mathbf{j}$ represent sources of the incoming fields in the scattering problem. The refractive index $n=n(\omega,\mathbf{x})$ can be both real or complex and can thus model both dielectrics and metals in the linear response regime. The fields are the frequency components $\mathbf{E}(\mathbf{x},\omega)$ and $\mathbf{B}(\mathbf{x},\omega)$ of the time-dependent $\mathbf{E}$ and $\mathbf{B}$ fields. Note that we use a sign convention where there is a minus sign in the exponent of the inverse Fourier transform.

Let V_j for $j=1,2,\ldots,q$ be q homogeneous scattering regions with bounding surfaces S_j, these are usually compact domains. Furthermore, let V_0 be the region exterior to all the objects V_j, this is usually a noncompact domain. The Müller scattering equations for this situation are given by

$$\begin{aligned} n_j^2\mathbf{E}_j^-(\xi)+n_0^2\mathbf{E}_0^+(\xi) &= 2n_0^2\mathbf{E}^i(\xi)-2\int_{S_j}\big\{\mathrm{i}k_0c(\mathbf{B}_j^+\times\mathbf{n})\\ &\quad\cdot(n_j^2G_j-n_0^2G_0)+(\mathbf{E}_j^+\times\mathbf{n})\cdot(\nabla\times(n_j^2G_j-n_0^2G_0))\big\}\,\mathrm{d}S\\ &\quad+2\sum_{l\neq j}\int_{S_l}\big\{\mathrm{i}k_0c(\mathbf{B}_l^+\times\mathbf{n})\cdot(n_0^2G_0)\\ &\quad+(\mathbf{E}_l^+\times\mathbf{n})\cdot(\nabla\times(n_0^2G_0))\big\}\,\mathrm{d}S \end{aligned} \tag{1}$$

$$\begin{aligned} \mathbf{B}_j^-(\xi)+\mathbf{B}_j^+(\xi) &= 2\mathbf{B}^i(\xi)-2\int_{S_j}\bigg\{-\mathrm{i}\frac{k_0}{c}(\mathbf{E}_l^+\times\mathbf{n})\\ &\quad\cdot(n_j^2G_j-n_0^2G_0)+(\mathbf{B}_l^+\times\mathbf{n})\cdot(\nabla\times(G_j-G_0))\bigg\}\,\mathrm{d}S\\ &\quad+2\sum_{l\neq j}\int_{S_l}\bigg\{-\mathrm{i}\frac{k_0}{c}(\mathbf{E}_l^+\times\mathbf{n})\cdot(n_0^2G_0)+(\mathbf{B}_l^+\times\mathbf{n})\cdot(\nabla\times G_0)\bigg\}\,\mathrm{d}S. \end{aligned} \tag{2}$$

In these integral equations, $k_0=\frac{\omega}{c}$ and ξ is an arbitrary point on the surfaces S_j. The quantities $\mathbf{E}_j^-$ and $\mathbf{B}_j^-$ are the electric and magnetic fields evaluated infinitesimally close to the inside of the bounding surface S_j, and $\mathbf{E}_j^+$ and $\mathbf{B}_j^+$ are the fields evaluated infinitesimally close to the outside of the bounding surface S_j.

The fields $\mathbf{E}^i$ and $\mathbf{B}^i$ are the electric and magnetic fields generated by the source in the absence of any scattering object. These are by definition the incoming fields in scattering theory. The matrix-valued quantities $G_j(\mathbf{x},\xi)$ are the dyadic Green's functions for the Maxwell equations in regions of constant refractive index:

$$G_j(\mathbf{x},\xi)=g_j(\mathbf{x},\xi)I+\left(\frac{1}{k_0^2n_j^2}\right)\nabla\nabla g_j(\mathbf{x},\xi),$$

where I is the identity matrix and $g_j(\mathbf{x},\xi)$ is the following Green's function for the vector Helmholtz equation:

$$g_j(\mathbf{x},\xi)=-\frac{\mathrm{e}^{\mathrm{i}k_0n_j\|\mathbf{x}-\xi\|}}{4\pi\|\mathbf{x}-\xi\|}.$$

Note that, for $l=j$, the surface integrals are Cauchy principal value integrals since the dyadic Green's function has a singularity when $\mathbf{x}=\xi$.

Using the fact that the magnetic field and the tangential component of the electric field are continuous across an interface between nonmagnetic materials and that the normal component of the electric field satisfies

$$(n_0^2\mathbf{E}_j^+-n_j^2\mathbf{E}_j^-)\cdot\mathbf{n}=0,$$

$\mathbf{E}_j^-$ and $\mathbf{B}_j^-$ can be eliminated and we have a closed system of equations that can be solved for the surface field values $\mathbf{E}_j^+$ and $\mathbf{B}_j^+$. The equations can be considerably simplified by decomposing the fields into tangential and normal components:

$$\begin{aligned}
\varphi_i&=(\mathbf{E}\times\mathbf{n})|_{S_i} & \varphi_i^i&=\frac{2n_0^2}{n_i^2+n_0^2}(\mathbf{E}^i\times\mathbf{n})|_{S_i},\\
\psi_i&=(\mathbf{B}\times\mathbf{n})|_{S_i} & \psi_i^i&=(\mathbf{B}^i\times\mathbf{n})|_{S_i},\\
u_i&=(\mathbf{B}\cdot\mathbf{n})|_{S_i} & u_i^i&=(\mathbf{B}^i\cdot\mathbf{n})|_{S_i},\\
v_i&=(\mathbf{E}\cdot\mathbf{n})|_{S_i} & v_i^i&=(\mathbf{E}^i\cdot\mathbf{n})|_{S_i}.
\end{aligned}$$

The resulting system of integral equations is as follows:

$$\varphi_i(\xi)=\varphi_i^i(\xi)+\sum_k\int_{S_k}\{\varphi_k(\mathbf{x})\cdot K_{ik}(\xi,\mathbf{x})+\psi_k(\mathbf{x})\cdot L_{ik}(\xi,\mathbf{x})\}\,\mathrm{d}S,\qquad(3)$$

$$\psi_i(\xi)=\psi_i^i(\xi)+\sum_k\int_{S_k}\{\varphi_k(\mathbf{x})\cdot P_{ik}(\xi,\mathbf{x})+\psi_k(\mathbf{x})\cdot Q_{ik}(\xi,\mathbf{x})\}\,\mathrm{d}S,\qquad(4)$$

$$u_i(\xi)=u_i^i(\xi)+\sum_k\int_{S_k}\{\varphi_k(\mathbf{x})\cdot M_{ik}(\xi,\mathbf{x})+\psi_k(\mathbf{x})\cdot N_{ik}(\xi,\mathbf{x})\}\,\mathrm{d}S,$$

$$v_i(\xi)=v_i^i(\xi)+\sum_k\int_{S_k}\{\varphi_k(\mathbf{x})\cdot R_{ik}(\xi,\mathbf{x})+\psi_k(\mathbf{x})\cdot S_{ik}(\xi,\mathbf{x})\}\,\mathrm{d}S,$$

where

$$L_{ik}(\xi,\mathbf{x})=-\frac{2\mathrm{i}k_0c}{n_i^2+n_0^2}(n_k^2G_k(\xi,\mathbf{x})-n_0^2G_0(\xi,\mathbf{x})),\qquad(5)$$

etc. We note that the normal components are decoupled from the tangential components. The computational strategy is to first solve the equations for the tangential components, thereafter compute the normal components from the two last equations and finally reconstruct the electric and magnetic fields using the relations

$$\mathbf{E}(\xi)=u(\xi)\mathbf{n}(\xi)+\mathbf{n}(\xi)\times\varphi(\xi),$$

$$\mathbf{B}(\xi)=v(\xi)\mathbf{n}(\xi)+\mathbf{n}(\xi)\times\psi(\xi).$$

3. Numerical implementation

We discretize the Müller scattering equations by splitting each surface into a large number of disjoint parts

$$S_i=\cup_jS_{ij}$$

and by selecting a corresponding collection of points ξ_{ij} with $\xi_{ij}\in S_{ij}$. The scattering equations (3) and (4) are required to hold at the collection of points ξ_{ij}. Therefore,

$$\varphi_{ij}=\varphi_{ij}^i+\sum_{kl}\int_{S_{kl}}\left\{\varphi_k(\mathbf{x})\cdot K_{ik}(\xi_{ij},\mathbf{x})+\psi_k(\mathbf{x})\cdot L_{ik}(\xi_{ij},\mathbf{x})\right\}\mathrm{d}S,$$

$$\psi_{ij}=\psi_{ij}^i+\sum_{kl}\int_{S_{kl}}\left\{\varphi_k(\mathbf{x})\cdot P_{ik}(\xi_{ij},\mathbf{x})+\psi_k(\mathbf{x})\cdot Q_{ik}(\xi_{ij},\mathbf{x})\right\}\mathrm{d}S,$$

where $\varphi_{ij}=\varphi_i(\xi_{ij})$ and $\psi_{ij}=\psi_i(\xi_{ij})$. A simple approximation scheme for the terms in the sums is

$$\int_{S_{kl}}\psi_k(\mathbf{x})\cdot L_{ik}(\xi_{ij},\mathbf{x})\mathrm{d}S\approx\psi_{kl}\cdot L_{ijkl},$$

where the tensor L_{ijkl} is defined by

$$L_{ijkl}=\int_{S_{kl}}L_{ik}(\xi_{ij},\mathbf{x})\,\mathrm{d}S.$$

The same approximation applied to the other terms in the scattering equations gives us a set of linear algebraic equations:

$$\begin{aligned}
\varphi_{ij}&=\varphi_{ij}^i+\sum_{kl}\left\{\varphi_{kl}\cdot K_{ijkl}+\psi_{kl}\cdot L_{ijkl}\right\},\\
\psi_{ij}&=\psi_{ij}^i+\sum_{kl}\left\{\varphi_{kl}\cdot P_{ijkl}+\psi_{kl}\cdot Q_{ijkl}\right\}.
\end{aligned}\qquad(6)$$

For terms where $(i,j)\neq(k,l)$, we use a 2D Gauss quadrature. For terms with $(i,j)=(k,l)$, which are the diagonal terms, the integrand has a singularity in the integration domain and the integrals must be solved as a 2D principal value integral. This means that if D_ε is a circular disc of radius ε centred on the point ξ_{kl}, then by definition

$$L_{ijij}=\lim_{\varepsilon\longrightarrow0}\int_{S_{ij}-D_\varepsilon}L_{ij}(\xi_{ij},\mathbf{x})\,\mathrm{d}S.$$

It follows from the construction of the Müller scattering equations that all such principal value integrals exist and thus the diagonal terms are finite. The diagonal terms are calculated by using a further approximation that reduces them to line integrals around the boundary of the surface S_{ij}. We illustrate how this is done by using the tensor L_{ijij}. Some simple algebra gives

$$L_{ijij} = -\frac{2ik_0c}{n_i^2+n_0^2}\left(\left[\lim_{\varepsilon\longrightarrow 0}\int_{S_{ij}-D_\varepsilon}\alpha(r)\mathrm{d}S\right]I + \left[\lim_{\varepsilon\longrightarrow 0}\int_{S_{ij}-D_\varepsilon}\frac{\beta(r)}{r^2}\mathbf{rr}\mathrm{d}S\right]\right), \quad (7)$$

where $\mathbf{r}=\mathbf{x}-\xi_{ij}$, $r=\|\mathbf{r}\|$ and $\alpha(r)$, $\beta(r)$ are certain functions with a singularity at $r=0$ that are derived from the dyadic Green's function. We now assume that the surface pieces S_{ij} are taken to be so small that they can be assumed to be flat. The integrals in (7) are then integrals in a plane with coordinate vector $\mathbf{r}=(x, y)$ and can be simplified by using a version of Green's theorem for plane regions. Note that we have the following identities:

$$\nabla\cdot(g(r)\mathbf{r}) = \alpha(r),$$
$$\nabla\cdot(h(r)\mathbf{rrr}) = \frac{\beta(r)}{r^2}\mathbf{rr},$$

where

$$g(r) = \frac{1}{r^2}\int_0^r r'\alpha(r')\,\mathrm{d}r',$$
$$h(r) = \frac{1}{r^4}\int_0^r r'\beta(r')\,\mathrm{d}r'.$$

Green's theorem gives

$$\lim_{\varepsilon\longrightarrow 0}\int_{S_{ij}-D_\varepsilon}\alpha(r)\,\mathrm{d}S = \int_{\partial S_{ij}} g(r)\mathbf{r}\cdot\mathbf{n}\mathrm{d}l + \lim_{\varepsilon\longrightarrow 0}\int_{\partial D_\varepsilon} g(r)\mathbf{r}\cdot\mathbf{n}\mathrm{d}l = \int_{\partial S_{ij}} g(r)\mathbf{r}\cdot\mathbf{n}\mathrm{d}l,$$

$$\lim_{\varepsilon\longrightarrow 0}\int_{S_{ij}-D_\varepsilon}\frac{\beta(r)}{r^2}\mathbf{rr}\mathrm{d}S = \int_{\partial S_{ij}} h(r)\mathbf{rrr}\cdot\mathbf{n}\mathrm{d}l + \lim_{\varepsilon\longrightarrow 0}\int_{\partial D_\varepsilon} h(r)\mathbf{rrr}\cdot\mathbf{n}\mathrm{d}l = \int_{\partial S_{ij}} h(r)\mathbf{rrr}\cdot\mathbf{n}\mathrm{d}l.$$

The integrals defining the functions $g(r)$ and $h(r)$ can be solved in terms of elementary functions. The line integrals around the boundary of S_{ij} are solved numerically using Gauss quadrature. The linear system (6) is nonsparse and nonhermitean as is typical for the BIM. However, the linear system is rather small (a few thousand equations for micronsized spheres) and is effectively solved by using the generalized minimum residual method (GMRES) [16]. We use a parallel implementation of GMRES developed by CERFACS [7].

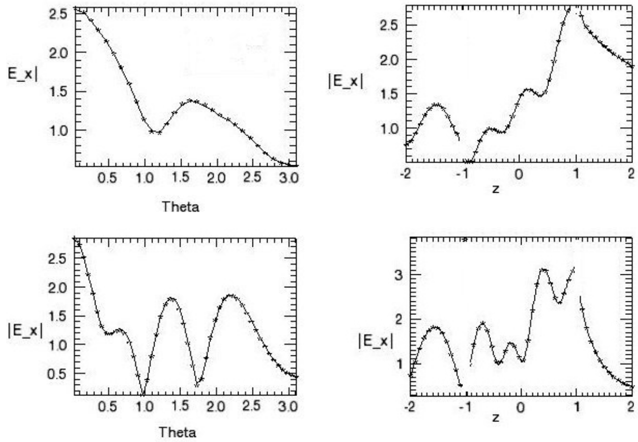

Figure 1. BIM solution (line) and Mie solution (crosses) for the electric field of a single sphere of index $n = 1.5$ and 2.0.

4. Validation of numerical implementation

Considering the mathematical status of the derivation of the Müller scattering equations and various approximations used in deriving the linear algebraic system, it is important to solve the equations for cases where exact solutions are known or where the scattering problem has been solved by other means. This will give an indication of the accuracy of the assumed approximations.

4.1. Single spheres

We start with the classical case of a plane wave scattering off a dielectric or metallic sphere. The exact solution is the well-known Mie solution [4]. We assume that the plane wave is polarized along the x-axis and that the wave vector points along the positive z-axis. In figure 1, the exact solution is compared with the boundary integral solution for a sphere of diameter $2\,\mu$m and with the incoming light having a wavelength of $2\,\mu$m. In the first row of figure 1, the sphere has an index 1.5 and in the second row it has an index 2.0. The index of the surrounding medium is in all cases 1.0. In the left column of the figure, we compare the x-components of the amplitude of the electric field $|E_x|$ that are infinitesimally close to the outside of the sphere along a longitude of the sphere. Theta is the longitudinal angle with respect to the positive z-axis. The angle of latitude with respect to the positive x-axis is 0 in this figure. The Mie solution is always represented by crosses and the boundary integral solution by lines. In the right column, we compare $|E_x|$ along the z-axis. We compute the field along the axis using the following integral relations:

$$\mathbf{E}(\xi) = \mathbf{E}^i(\xi) + \int_S \left\{ik_0c(\mathbf{B}^+\times\mathbf{n})\cdot G_0 + (\mathbf{E}^+\times\mathbf{n})\cdot(\nabla\times G_0)\right\}\mathrm{d}S, \quad (8)$$

$$\mathbf{E}(\xi) = -\int_{S_j}\{ik_0c(\mathbf{B}_j^-\times\mathbf{n})\cdot G_j + (\mathbf{E}_j^-\times\mathbf{n})\cdot(\nabla\times G_j)\}\mathrm{d}S, \quad (9)$$

where equation (9) is applied inside the sphere and (8) outside the sphere. Note that there is a break in the curves for the on-axis fields where they cross the sphere surface. This is because equations (8) and (9) have nonintegrable singularities

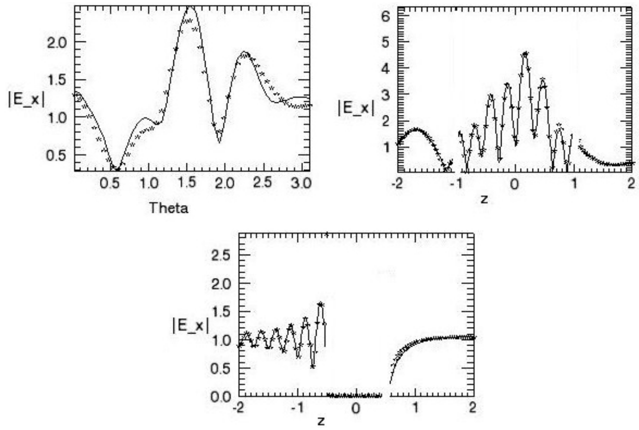

Figure 2. BIM solution (lines) and Mie solution (crosses) for the electric field of a single sphere of index $n = 4$ (top) and $2.0 + \mathrm{i}7.0$ (bottom).

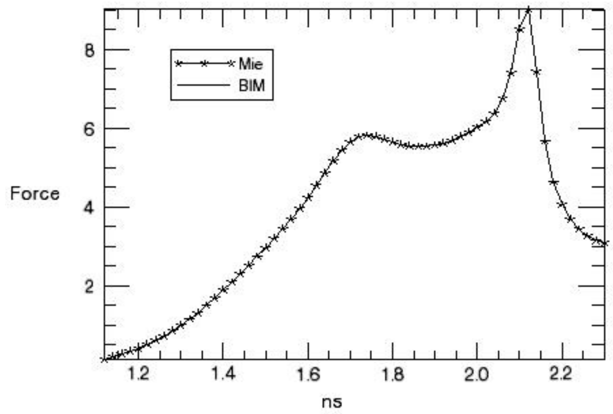

Figure 3. Force on a single sphere as a function of index. BIM solution (line) and Mie solution (crosses).

at the surface. If for some reason values of the electromagnetic field close to but not infinitesimally close to the surface are needed, there will be a direct relation between the distance to the sphere surface and the number of points we must use in the discretization of the boundary integral equations. It is important to note that the singularities in (8) and (9) play no role in the calculations of forces and resonance curves as such calculations only depend on the fields that are infinitesimally close to the surface. In figure 2, the first row has the same interpretation as that in figure 1 but here the index of the sphere is 4. In the lower row, we compare the field along the z-axes for a small aluminum sphere of radius 0.24 μm with incoming light of wavelength 0.65 μm.

The figures show that our implementation of the boundary integral equations is quite accurate. Only for a sphere index of 4.0 is there any noticeable difference, and the difference is small. In figure 3, we compare the z-component of the optical force computed using the Mie solution and the boundary integral equations for a range of indices for the sphere. The Mie solution is as usual represented by crosses.

4.2. Two concentric spheres

The scattering problem for two concentric spheres has been solved by using the same approach as in the single sphere case [1]. The Müller scattering equations (1) and (2) were derived under the assumption that the scattering objects have zero intersection. For the case when we have inclusion relations between the scattering objects, the scattering equations are derived using the same approach, but the equations will be slightly different. If scattering object no. 1 with index n_1 is included in scattering object no. 2 with index n_2 and if the outside of object no. 2 has index n_0, the equations are found to be

$$n_1^2\mathbf{E}_1^-(\xi) + n_2^2\mathbf{E}_1^+(\xi) = -2\int_{S_1}\left\{\mathrm{i}k_0c(\mathbf{B}_1^+\times\mathbf{n})\cdot(n_1^2G_1 - n_2^2G_2)\right.$$

$$\left.+(\mathbf{E}_1^+\times\mathbf{n})\cdot(\nabla\times(n_1^2G_1 - n_2^2G_2))\right\}\mathrm{d}S$$

$$-2\int_{S_2}\left\{\mathrm{i}k_0c(\mathbf{B}_2^+\times\mathbf{n})\cdot(n_2^2G_2) + (\mathbf{E}_2^+\times\mathbf{n})\cdot(\nabla\times(n_2^2G_2))\right\}\mathrm{d}S,$$

$$n_2^2\mathbf{E}_2^-(\xi) + n_0^2\mathbf{E}_2^+(\xi) = 2n_0^2\mathbf{E}^i(\xi)$$

$$-2\int_{S_2}\left\{\mathrm{i}k_0c(\mathbf{B}_2^+\times\mathbf{n})\cdot(n_2^2G_2 - n_0^2G_0)\right.$$

$$\left.+(\mathbf{E}_2^+\times\mathbf{n})\cdot(\nabla\times(n_2^2G_2 - n_0^2G_0))\right\}\mathrm{d}S$$

$$+2\int_{S_1}\left\{\mathrm{i}k_0c(\mathbf{B}_1^+\times\mathbf{n})\cdot(n_2^2G_2) + (\mathbf{E}_1^+\times\mathbf{n})\cdot(\nabla\times(n_2^2G_2))\right\}\mathrm{d}S,$$

$$\mathbf{B}_1^-(\xi) + \mathbf{B}_1^+(\xi) = -2\int_{S_1}\left\{-\mathrm{i}\frac{k_0}{c}(\mathbf{E}_1^+\times\mathbf{n})\cdot(n_1^2G_1 - n_2^2G_2)\right.$$

$$\left.+(\mathbf{B}_1^+\times\mathbf{n})\cdot(\nabla\times(G_1 - G_2))\right\}\mathrm{d}S$$

$$-2\int_{S_2}\left\{-\mathrm{i}\frac{k_0}{c}(\mathbf{E}_2^+\times\mathbf{n})\cdot(n_2^2G_2) + (\mathbf{B}_2^+\times\mathbf{n})\cdot(\nabla\times(G_2))\right\}\mathrm{d}S,$$

$$\mathbf{B}_2^-(\xi) + \mathbf{B}_2^+(\xi) = -2\int_{S_2}\left\{-\mathrm{i}\frac{k_0}{c}(\mathbf{E}_2^+\times\mathbf{n})\cdot(n_2^2G_1 - n_0^2G_0)\right.$$

$$\left.+(\mathbf{B}_2^+\times\mathbf{n})\cdot(\nabla\times(G_2 - G_0))\right\}\mathrm{d}S$$

$$+2\int_{S_1}\left\{-\mathrm{i}\frac{k_0}{c}(\mathbf{E}_1^+\times\mathbf{n})\cdot(n_2^2G_2) + (\mathbf{B}_1^+\times\mathbf{n})\cdot(\nabla\times(G_0))\right\}\mathrm{d}S.$$

The equations are solved for a fixed value, $n_1 = 4$, of the index of the inner sphere and a range of values from 1.0 to 4.0 of the index n_2 of the outer sphere. The result is shown in figure 4. The figure shows that for most values of the outer index, the forces calculated by using the Mie solution and the boundary integral solution are quite close. The enhanced values of the force occur as expected at Mie resonances for two concentric spheres. The actual error is a few percent for most values of the outer index.

Comparison between a purely serial implementation and a coarse grained parallel implementation running on four cores shows a speedup by a factor of 3. This large speedup is a result of the fact that in the boundary integral approach to solving the Maxwell equations, a large fraction of the work goes into calculating the matrix elements, and this part of the calculation is trivially 100% parallelizable. The scaling behavior of our algorithm for solving the Müller scattering equations was further investigated by implementing the algorithm on a large cluster. The following table shows

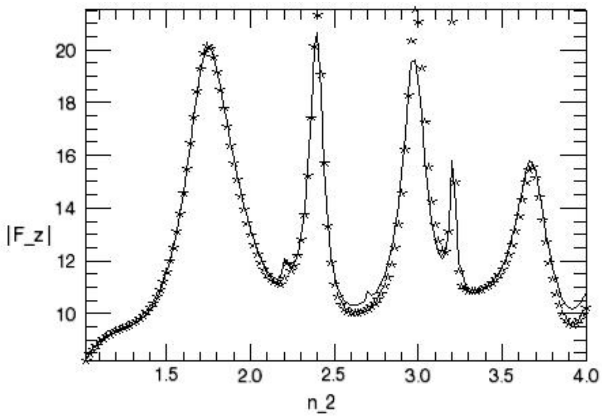

Figure 4. Force on a layered sphere as a function of the index of the outer layer. BIM solution (line) and Mie solution (crosses).

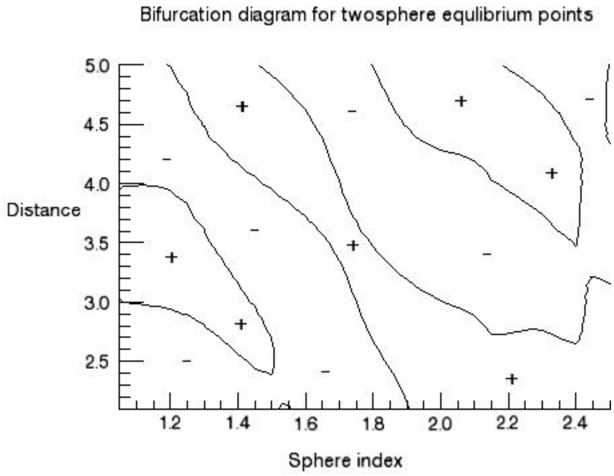

Figure 5. Bifurcation diagram for two sphere equilibrium points.

the execution times on the cluster for N randomly placed dielectric spheres. The spheres have a radius of $1\,\mu$m and a refractive index of $n = 2$. The resolution is 1800 points per sphere.

N	Running times (s)	#cpu
1	45	2
2	65	5
3	68	10
4	70	17
5	71	26
6	73	37
7	90	50
9	105	82
12	119	145

Few, if any, algorithms for solving the Maxwell equations can match this efficiency.

5. Force between a pair of dielectric spheres

There have been a fair number of experimental and theoretical investigations of the force between two dielectric spheres in the field generated by two incoherent counter propagating laser beams. In particular, the location and stability of force equilibrium points have been of interest. In [12], the system consisting of two spheres oriented along the axis of the two counter propagating beams was investigated. The index step between the spheres and the host (sugar water) was chosen to be small in order to ensure that the light scattering properties of the system could be described within the paraxial approximation. This made it possible to simulate the system by using a standard beam propagating code. The simulation compared well with the experiment and both showed the existence of a bifurcation diagram with up to three force equilibria for variable index steps. The same system was investigated in [10]. Here the system was simulated using the coupled dipole method (CDM). This method does not depend on the paraxial approximation and is in principle exact. In practice, many of the same numerical issues arise as in the BIM. Discretization typically leads to matrices that are much larger than for the BIM for a fixed accuracy and this is obviously an issue when linear systems are to be solved. The CDM shows that backscattering is important and leads to the existence of multiple closely spaced force equilibria that makes comparison with the experiment difficult, as noted by the authors in [10].

The effect of the backscatter can be avoided and cleaner results can be obtained if the location of the source lasers is rotated by 90° so that the beam is perpendicular to the axis connecting the centers of the spheres. One should of course defocus the beam such that any source-induced gradient force effect is avoided and the measured forces are induced by light scattering alone. In figure 5, we show a sample bifurcation diagram for such a system computed by using the BIM. We assume a single plane wave source polarized along the axis connecting the centers of the two spheres, a background index of 1.0, two spheres with diameter $2\,\mu$m and a wavelength of $2\,\mu$m for the incoming plane wave. A plus sign in a region indicates that the spheres are attracted to each other and a minus sign indicates that they are repelled. As we can see from the diagram, there is a clear indication of the existence of the three equilibria and regions of bistability. It is evident that the geometry discussed here gives a better chance of comparison between experiment and computation than the setup discussed in [12] and [10].

6. Summary

In this paper, we have shown that the BIM is an effective and accurate computational method for solving a range of problems that are common in computational photonics. For solving these types of problems, we believe that none of the standard domain-based methods can compete with the BIM with respect to efficiency and implementational simplicity, especially in a parallel cluster-based computational environment. The method has been tested on single spheres and concentric spheres where exact solutions are available and has been used to predict bistability for two spheres with a geometry that differs from the one that was discussed previously. This last result is, as far as we know, new.

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Appendix

The boundary integral formulation of the Maxwell equations used in this paper is usually called the Müller scattering equations. The actual derivation of these equations is however not easy to find in the literature and we therefore consider it appropriate to include a detailed description of the regularization procedure in this appendix to the paper. Other boundary integral formulations of the 3D Maxwell equations can be found in the literature [6], but we believe that for the calculation of optical forces the Müller scattering equations are the best choice. It is formulated directly in terms of the quantities of interest for force calculations, represents the singularity in an explicit way in terms of principal value integrals and is very efficient in the sense that for N discretization elements we have $4N$ equations to solve.

In order to derive the Müller scattering equations, we need a version of the second Green's identity. For a vector field φ and a matrix field A, we have the following for an arbitrary volume V with boundary ∂V:

$$\int_V \{(\nabla\times(\nabla\times\varphi))\cdot A-\varphi\cdot(\nabla\times(\nabla\times A))\}\,\mathrm{d}V$$
$$=\int_{\partial V}\mathbf{n}\cdot\{(\nabla\times\varphi)\times A+\varphi\times(\nabla\times A)\}\,\mathrm{d}S.$$

The second major ingredient we need is the fundamental solution $G(\mathbf{x},\xi)$ of the operator $L(\varphi)=-\nabla\times\nabla\times\varphi+k_0n^2\varphi$, corresponding to outgoing waves at infinity. With our sign convention for the Fourier transform, this is

$$G(\mathbf{x},\xi)=g(\mathbf{x},\xi)I+\left(\frac{1}{k_0^2n^2}\right)\nabla\nabla g(\mathbf{x},\xi),$$

where I is the identity matrix and $g(\mathbf{x},\xi)$ is a fundamental solution for the vector Helmholtz equation, given as

$$g(\mathbf{x},\xi)=-\frac{\mathrm{e}^{\mathrm{i}k_0n\|\mathbf{x}-\xi\|}}{4\pi\|\mathbf{x}-\xi\|}.$$

The matrix function $G(\mathbf{x},\xi)$ is a well-known dyadic Green's function and satisfies by constructing the equation

$$-\nabla\times\nabla\times G+k_0n^2G=\delta(\mathbf{x}-\xi)I,$$
$$\nabla\cdot G=0,\quad \mathbf{x}\neq\xi.$$

Using $\varphi=\mathbf{E}$ and $A=G$ in the vector–matrix Green's identity, we obtain the following by using the equations $L\mathbf{E}=\mathbf{j}_E$ and $LG=\delta(\mathbf{x}-\xi)I$.

$$\int_V \mathbf{E}(\mathbf{x})\delta(\mathbf{x}-\xi)\mathrm{d}V=\mathbf{E}^i(\xi)+\int_{\partial V}\mathbf{n}\cdot\{(\nabla\times\mathbf{E})\times G$$
$$+\mathbf{E}\times(\nabla\times G)\}\,\mathrm{d}S,$$

where we have defined

$$\mathbf{E}^i(\xi)=\int_V G\cdot\mathbf{j}_E\mathrm{d}V.$$

If we assume $\xi\in V$, we obtain the following fundamental integral identity for the electromagnetic field:

$$\mathbf{E}(\xi)=\mathbf{E}^i(\xi)+\int_{\partial V}\mathbf{n}\cdot\{(\nabla\times\mathbf{E})\times G+\mathbf{E}\times(\nabla\times G)\}\,\mathrm{d}S.$$

Using the Maxwell equations and some standard vector calculus, the integral identity can be written as

$$\mathbf{E}(\xi)=\mathbf{E}^i(\xi)-\int_{\partial V}\{\mathrm{i}k_0c(\mathbf{B}\times\mathbf{n})\cdot G+(\mathbf{E}\times\mathbf{n})\cdot(\nabla\times G)\}\,\mathrm{d}S.$$

In a similar way we obtain for the magnetic field

$$\mathbf{B}(\xi)=\mathbf{B}^i(\xi)-\int_{\partial V}\left\{-\mathrm{i}\frac{kn^2}{c}(\mathbf{E}\times\mathbf{n})\cdot G\right.$$
$$\left.+(\mathbf{B}\times\mathbf{n})\cdot(\nabla\times G)\right\}\mathrm{d}S.$$

In these two equations ξ is an arbitrary point inside the volume V. Note however that the equation for the dyadic Green's function holds for all ξ, also those that are not inside the volume V. Assuming ξ is outside the volume, we obtain two additional integral identities that play a crucial role in the derivation of the Müller scattering equations:

$$0=\mathbf{E}^i(\xi)-\int_{\partial V}\{\mathrm{i}k_0c(\mathbf{B}\times\mathbf{n})\cdot G+(\mathbf{E}\times\mathbf{n})\cdot(\nabla\times G)\}\,\mathrm{d}S,$$

$$0=\mathbf{B}^i(\xi)-\int_{\partial V}\left\{-\mathrm{i}\frac{kn^2}{c}(\mathbf{E}\times\mathbf{n})\cdot G+(\mathbf{B}\times\mathbf{n})\cdot(\nabla\times G)\right\}\mathrm{d}S.$$

These last two integral identities express what is traditionally called the Oseen extinction theorem and is the solution to a historically important problem concerned with the behavior of electromagnetic waves when they cross a boundary between two materials with different refractive indices. Note that the only assumptions involved in deriving the integral identities are that the field satisfy the stationary Maxwell equations inside the volume V, where the refractive index n is constant.

Let V_j for $j=1,2,\ldots,q$ be q homogeneous scattering regions with bounding surfaces S_j; these are usually compact domains. Furthermore, let V_0 be the region exterior to all the objects V_j; this is usually a noncompact domain. From the general integral identities for the electromagnetic field we obtain

$$\mathbf{E}(\xi)=-\int_{S_j}\left\{\mathrm{i}k_0c(\mathbf{B}_j^-\times\mathbf{n})\cdot G_j+(\mathbf{E}_j^-\times\mathbf{n})\cdot(\nabla\times G_j)\right\}\mathrm{d}S,$$

$$0=\mathbf{E}^i(\xi)+\sum_{l=1}^{q}\int_{S_l}\left\{\mathrm{i}k_0c(\mathbf{B}_l^+\times\mathbf{n})\cdot G_0\right.$$
$$\left.+(\mathbf{E}_l^+\times\mathbf{n})\cdot(\nabla\times G_0)\right\}\mathrm{d}S$$

for $\xi \in V_j$ with $j = 1, 2, \ldots, q$. For $\xi \in V_0$, we get the integral identities

$$\mathbf{E}(\xi) = \mathbf{E}^i(\xi) + \sum_{l=1}^{q} \int_{S_l} \left\{ \mathrm{i}k_0 c(\mathbf{B}_l^+ \times \mathbf{n}) \cdot G_0 + (\mathbf{E}_l^+ \times \mathbf{n}) \cdot (\nabla \times G_0) \right\} \mathrm{d}S,$$

$$0 = -\int_{S_j} \left\{ \mathrm{i}k_0 c(\mathbf{B}_j^- \times \mathbf{n}) \cdot G_j + (\mathbf{E}_j^- \times \mathbf{n}) \cdot (\nabla \times G_j) \right\} \mathrm{d}S,$$

where as usual the bounding surface at infinity gives no contribution. Here $\mathbf{E}_j^-$ and $\mathbf{B}_j^-$ are the electric and magnetic fields evaluated infinitesimally close to the inside of the bounding surface S_j, and $\mathbf{E}_j^+$ and $\mathbf{B}_j^+$ are the fields evaluated infinitesimally close to the outside of the bounding surface S_j. The function G_j is the dyadic Green's function in a homogeneous region with constant index n_j. In an exactly analogous manner, we obtain from the magnetic integral identities the following relations:

$$\mathbf{B}(\xi) = -\int_{S_j} \left\{ -\mathrm{i}\frac{k_0 n_j^2}{c} (\mathbf{E}_j^- \times \mathbf{n}) \cdot G_j + (\mathbf{B}_j^- \times \mathbf{n}) \cdot (\nabla \times G_j) \right\} \mathrm{d}S,$$

$$0 = \mathbf{B}^i(\xi) + \sum_{l=1}^{q} \int_{S_l} \left\{ -\mathrm{i}\frac{k_0 n_l^2}{c} (\mathbf{E}_l^+ \times \mathbf{n}) \cdot G_0 + (\mathbf{B}_l^+ \times \mathbf{n}) \cdot (\nabla \times G_0) \right\} \mathrm{d}S,$$

for $\xi \in V_j$ with $j = 1, 2, \ldots, q$. For $\xi \in V_0$, we obtain the integral identities

$$\mathbf{B}(\xi) = \mathbf{B}^i(\xi) + \sum_{l=1}^{q} \int_{S_l} \left\{ -\mathrm{i}\frac{k_0 n_l^2}{c} (\mathbf{E}_l^+ \times \mathbf{n}) \cdot G_0 + (\mathbf{B}_l^+ \times \mathbf{n}) \cdot (\nabla \times G_0) \right\} \mathrm{d}S,$$

$$0 = -\int_{S_j} \left\{ -\mathrm{i}\frac{k_0 n_j^2}{c} (\mathbf{E}_j^- \times \mathbf{n}) \cdot G_j + (\mathbf{B}_j^- \times \mathbf{n}) \cdot (\nabla \times G_j) \right\} \mathrm{d}S.$$

The fields $\mathbf{E}^i$ and $\mathbf{B}^i$ are defined as

$$\mathbf{E}^i(\xi) = \int_{V_0} G_0 \cdot \mathbf{j}_E \mathrm{d}V,$$

$$\mathbf{B}^i(\xi) = \int_{V_0} G_0 \cdot \mathbf{j}_B \mathrm{d}V,$$

and are the electric and magnetic fields at ξ generated by the source in the absence of any scattering objects. This is by definition the incoming field in scattering theory. Note that the tangential components of both the electric and magnetic fields are continuous across the bounding surface S_j so that we can use $\mathbf{E}_j^+$ and $\mathbf{B}_j^+$ in all integral expressions.

It is easy to see either from the derivation of the integral identities or by direct differentiation under the integrals that any choice of the fields $\mathbf{E}_j^+$ and $\mathbf{B}_j^+$ whatsoever will, through the integral identities, produce electric and magnetic fields that satisfy the Maxwell equations at every point that is not on the bounding surfaces and the radiation condition at infinity. Naively, the physical solution to the scattering problem should be selected by requiring that the limit of the fields when we approach the bounding surfaces S_j from the inside and the outside should be equal to $\mathbf{E}_j^-$, $\mathbf{B}_j^-$, $\mathbf{E}_j^+$ and $\mathbf{B}_j^+$. The problem of regularization is that these limits do not exist because the integrand has a nonintegrable singularity on the surface when $\mathbf{x} = \xi$. The regularization proceeds in two steps. First, we recall that the inside and outside dyadic Green's functions at the bounding surface S_j are

$$G_j(\mathbf{x}, \xi) = g_j(\mathbf{x}, \xi) I + \left(\frac{1}{k_0^2 n_j^2} \right) \nabla\nabla g_j(\mathbf{x}, \xi),$$

$$G_0(\mathbf{x}, \xi) = g_0(\mathbf{x}, \xi) I + \left(\frac{1}{k_0^2 n_0^2} \right) \nabla\nabla g_0(\mathbf{x}, \xi).$$

The nonintegrability of the singularity at $\mathbf{x} = \xi$ arises from the last term in the two expressions. Inside the bounding surface S_j, we have two integral identities, one involving G_j and the other involving G_0. The first step in regularization consists of taking a linear combination of these two integral identities that cancels the most singular part in the dyadic Green's function. Doing this for both the magnetic field and the electric field for all bounding surfaces gives the following set of integral identities:

$$\begin{aligned} n_j^2 \mathbf{E}(\xi) = n_0^2 \mathbf{E}^i(\xi) &- \int_{S_j} \{\mathrm{i}k_0 c(\mathbf{B}_j^+ \times \mathbf{n}) \cdot (n_j^2 G_j - n_0^2 G_0) \\ &+ (\mathbf{E}_j^+ \times \mathbf{n}) \cdot (\nabla \times (n_j^2 G_j - n_0^2 G_0))\} \mathrm{d}S \\ &+ \sum_{l=1}^{q} \int_{S_l} \left\{ \mathrm{i}k_0 c(\mathbf{B}_l^+ \times \mathbf{n})(n_0^2 G_0) + (\mathbf{E}_l^+ \times \mathbf{n}) \cdot (\nabla \times (n_0^2 G_0)) \right\} \mathrm{d}S, \end{aligned}$$

$$\begin{aligned} \mathbf{B}(\xi) = \mathbf{B}^i(\xi) &- \int_{S_j} \left\{ -\mathrm{i}\frac{k_0}{c} (\mathbf{E}_l^+ \times \mathbf{n}) \cdot (n_j^2 G_j - n_0^2 G_0) + (\mathbf{B}_l^+ \times \mathbf{n}) \cdot (\nabla \times (G_j - G_0)) \right\} \mathrm{d}S \\ &+ \sum_{l=1}^{q} \int_{S_l} \left\{ -\mathrm{i}\frac{k_0}{c} (\mathbf{B}_l^+ \times \mathbf{n}) \cdot (n_0^2 G_0) + (\mathbf{E}_l^+ \times \mathbf{n}) \cdot (\nabla \times G_0) \right\} \mathrm{d}S \end{aligned}$$

that holds for all ξ that are not on the bounding surfaces. Since we are now cancelling the worst singularities, it is possible to get finite answers when ξ approach the bounding surfaces S_j. However, we must specify precisely how the limit is taken. Let ξ be a point on the bounding surface S_j and let $\xi^\varepsilon = \xi + \varepsilon \mathbf{a}$ be a straight line through ξ with direction along the vector $\mathbf{a}$ and where positive values of ε correspond to points inside the surface S_j.

Let D_ε be a disc of radius ε and center ξ on the surface, S_j and let S_ε be the rest of the surface, so that we have

$S_j = D_\varepsilon \cup S_\varepsilon$. Any surface integral over S_j can now evidently be split into a sum of two pieces, one over D_ε and one over the rest of the surface S_ε. When we let $\varepsilon \to 0$, the contribution over the disc D_ε will in the limit give a finite contribution that we compute by using an asymptotic expression for the integrand close to its singular point. The integral over S_ε will in the same limit by definition become the principal value integral at the point ξ on the surface. This gives us the following set of integral equations for the surface values of the electric and magnetic fields:

$$n_j^2\mathbf{E}_j^{\pm}(\xi) = n_0^2\mathbf{E}^i(\xi) - \int_{S_j}\{\mathrm{i}k_0c(\mathbf{B}_j^+\times\mathbf{n})\cdot(n_j^2G_j - n_0^2G_0) + (\mathbf{E}_j^+\times\mathbf{n})\cdot(\nabla\times(n_j^2G_j-n_0^2G_0))\}\mathrm{d}S + \sum_{l\neq j}\int_{S_l}\{\mathrm{i}k_0c(\mathbf{B}_l^+\times\mathbf{n})\cdot(n_0^2G_0) + (\mathbf{E}_l^+\times\mathbf{n})\cdot(\nabla\times(n_0^2G_0))\}\mathrm{d}S \mp \frac{n_j^2-n_0^2}{4\pi}E_{j\|}^+\cdot(\mathbf{bn}-(\mathbf{b}\cdot\mathbf{n})I),$$

$$\mathbf{B}_j^{\pm}(\xi) = \mathbf{B}^i(\xi) - \int_{S_j}\left\{-\mathrm{i}\frac{k_0n_j^2}{c}(\mathbf{E}_l^+\times\mathbf{n})\cdot(n_j^2G_j-n_0^2G_0) + (\mathbf{B}_l^+\times\mathbf{n})\cdot(\nabla\times(G_j-G_0))\right\}\mathrm{d}S + \sum_{l\neq j}\int_{S_l}\left\{-\mathrm{i}\frac{k_0}{c}(\mathbf{B}_l^+\times\mathbf{n})\cdot(n_0^2G_0) + (\mathbf{E}_l^+\times\mathbf{n})\cdot(\nabla\times G_0)\right\}\mathrm{d}S \mp \frac{n_j^2-n_0^2}{4\pi}\mathbf{B}_{j\|}^+\cdot(\mathbf{bn}-(\mathbf{b}\cdot\mathbf{n})I),$$

where $\mathbf{b}$ is a vector that depends on the vector $\mathbf{a}$ and the surface integrals are the principal value integrals. Now we come to the second part of the problem of regularization. The equations for the surface fields depend on the way the limit is taken and we are thus not directly able to select one unique solution to the scattering problem. The regularization is completed by noting that the limit-dependent term in the equations occurs with an opposite sign when we consider limits from the inside and the outside. Thus the limit-dependent terms can be cancelled if the limit $\varepsilon \to 0$ is taken of the sum of the inner and outer integral identities. This final step gives the Müller scattering equations:

$$n_j^2\mathbf{E}_j^-(\xi) + n_0^2\mathbf{E}_0^+(\xi) = 2n_0^2\mathbf{E}^i(\xi) - 2\int_{S_j}\{\mathrm{i}k_0c(\mathbf{B}_j^+\times\mathbf{n})\cdot(n_j^2G_j-n_0^2G_0) + (\mathbf{E}_j^+\times\mathbf{n})\cdot(\nabla\times(n_j^2G_j-n_0^2G_0))\}\mathrm{d}S + 2\sum_{l\neq j}\int_{S_l}\{\mathrm{i}k_0c(\mathbf{B}_l^+\times\mathbf{n})\cdot(n_0^2G_0) + (\mathbf{E}_l^+\times\mathbf{n})\cdot(\nabla\times(n_0^2G_0))\}\,\mathrm{d}S,$$

$$\mathbf{B}_j^-(\xi) + \mathbf{B}_j^+(\xi) = 2\mathbf{B}^i(\xi) - 2\int_{S_j}\left\{-\mathrm{i}\frac{k_0n_j^2}{c}(\mathbf{E}_l^+\times\mathbf{n})\cdot(n_j^2G_j-n_0^2G_0) + (\mathbf{B}_l^+\times\mathbf{n})\cdot(\nabla\times(G_j-G_0))\right\}\mathrm{d}S + 2\sum_{l\neq j}\int_{S_l}\left\{-\mathrm{i}\frac{k_0}{c}(\mathbf{B}_l^+\times\mathbf{n})\cdot(n_0^2G_0) + (\mathbf{E}_l^+\times\mathbf{n})\cdot(\nabla\times G_0)\right\}\mathrm{d}S.$$

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