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A fast multipole method for the three-dimensional Stokes equations

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Abstract

Many problems in Stokes flow (and linear elasticity) require the evaluation of vector fields defined in terms of sums involving large numbers of fundamental solutions. In the fluid mechanics setting, these are typically the Stokeslet (the kernel of the single layer potential) or the Stresslet (the kernel of the double layer potential). In this paper, we present a simple and efficient method for the rapid evaluation of such fields, using a decomposition into a small number of Coulombic *N*-body problems, following an approach similar to that of Fu and Rodin [Y. Fu, G.J. Rodin, Fast solution methods for three-dimensional Stokesian many-particle problems, Commun. Numer. Meth. En. 16 (2000) 145–149]. While any fast summation algorithm for Coulombic interactions can be employed, we present numerical results from a scheme based on the most modern version of the fast multipole method [H. Cheng, L. Greengard, V. Rokhlin, A fast adaptive multipole algorithm in three dimensions, J. Comput. Phys. 155 (1999) 468–498]. This approach should be of value in both the solution of boundary integral equations and multiparticle dynamics.

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1. Introduction

During the last two decades, a substantial body of work has emerged on fast algorithms for potential theory. The bulk of these have considered the Coulombic or gravitational *N*-body problem or the solution of related boundary integral equations. The *N*-body problem requires evaluations of sums on the form

$$F^{\mathsf{m}} = \sum_{\substack{n=1\\n\neq m}}^{N} \frac{f^{\mathsf{n}}}{\|\mathbf{x}^{\mathsf{n}} - \mathbf{x}^{\mathsf{m}}\|} + \sum_{\substack{n=1\\n\neq m}}^{N} \frac{(\hat{\mathbf{n}}^{\mathsf{n}} \cdot \mathbf{r}_{\mathsf{n}\mathsf{m}})g^{\mathsf{n}}}{\|\mathbf{x}^{\mathsf{n}} - \mathbf{x}^{\mathsf{m}}\|^{3}}, \quad \mathsf{m} = 1, \dots, N,$$
(1)

where $\mathbf{x}^{m}, \mathbf{x}^{n} \in \mathbb{R}^{3}$, $\hat{\mathbf{n}}^{n} \in \mathbb{R}^{3}$ is an arbitrary orientation vector, and $f^{n}, g^{n} \in \mathbb{R}$. A typical boundary integral equation takes the form

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$$F(\mathbf{x}) = a\sigma(\mathbf{x}) + b \int_{\Gamma} G(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})d\mathbf{y} + c \int_{\Gamma} \frac{\mathrm{d}}{\mathrm{d}n_{\mathbf{y}}} G(\mathbf{x}, \mathbf{y})\sigma(\mathbf{y})d\mathbf{y},$$
(2)

where Γ is a surface in \mathbb{R}^3 , $G(\mathbf{x}, \mathbf{y}) = 1/||\mathbf{x} - \mathbf{y}||$, $\frac{d}{dn_y}$ refers to the normal derivative at the point \mathbf{y} , and a, b, c are constants that depend on the particular boundary condition being imposed. In general, $F(\mathbf{x})$ is given as data and σ is an unknown surface density. In physical terms, the first sum in (1) is the field due to a collection of charges and the second sum is the field due to a collection of dipoles. Likewise, the first integral in (2) is the field due to a surface charge distribution (a single layer potential) and the second integral is the field due to a continuous distribution of normally oriented dipoles (a double layer potential). Discretizing the integrals in (2) by some quadrature rule, we obtain discrete sums over the quadrature points of the same form as (1).

In short, *N*-body calculations arise in two main contexts: the evaluation of particle interactions and the evaluation of layer potentials (often as part of the iterative solution of boundary integral equations). Since the governing equation is the Laplace equation, we will refer to these as harmonic *N*-body calculations.

The straightforward evaluation of F^m in (1) for m = 1, ..., N clearly requires $O(N^2)$ work. There are, however, a variety of fast algorithms that are capable of reducing that cost to O(N) or $O(N \log N)$. These include fast multipole methods, tree codes, the method of local corrections, multigrid methods, panel clustering methods, particle-in-cell methods, particle-mesh Ewald methods, and pre-corrected FFT methods. We will not attempt to review the literature on fast algorithms, but refer the reader to a few selected papers on the fast multipole method (FMM) [1,2,6,8,15], since it is the algorithm we will rely on here. It is worth noting, in the present context, that both particle-mesh-Ewald methods and pre-corrected FFT methods have been extended to the case of Stokes flow and used with great effect [10,13]. The principal advantage of the FMM is that it is fully adaptive, and handles highly inhomogeneous source distributions as easily as it does homogeneous ones. It has the disadvantage that it is much more complex to implement efficiently.

1.1. Stokeslets and Stresslets

In Stokes flow and linear elasticity, computations analogous to (1) arise naturally. Both involve vector versions of the *N*-body problem. In this short paper, we concentrate on the Stokes problem.

One fundamental solution for the Stokes equations is the Stokeslet

$$S_{ij}(\mathbf{x}, \mathbf{y}) = \frac{\delta_{ij}}{|\mathbf{x} - \mathbf{y}|} + \frac{(x_i - y_i)(x_j - y_j)}{|\mathbf{x} - \mathbf{y}|^3}, \quad i, j = 1, 2, 3,$$
(3)

where δ_{ij} is the Kronecker delta, $\mathbf{x} = (x_1, x_2, x_3)$ and $\mathbf{y} = (y_1, y_2, y_3)$. The corresponding summation problem is the calculation of the vector $\mathbf{F}^m = (F_1^m, F_2^m, F_3^m)$ at each source location \mathbf{x}^m from the formula

$$F_i^{\mathsf{m}} = \sum_{\substack{n=1\\n\neq \mathsf{m}}}^N \sum_{j=1}^3 S_{ij}(\mathbf{x}^{\mathsf{m}}, \mathbf{x}^{\mathsf{n}}) f_j^{\mathsf{n}}, \quad i = 1, 2, 3, \quad \mathsf{m} = 1, \dots, N,$$
(4)

where $\{\mathbf{f}^n = (f_1^n, f_2^n, f_3^n)\}$ are the vector source strengths. A second fundamental solution is the Stresslet

$$D_{ij}(\mathbf{x}, \mathbf{y}, \hat{\mathbf{n}}) = \sum_{k=1}^{3} \frac{(x_i - y_i)(x_j - y_j)(x_k - y_k)\hat{n}_k}{|\mathbf{x} - \mathbf{y}|^5},$$
(5)

with $\hat{\mathbf{n}} \in \mathbb{R}^3$ an orientation vector. The corresponding summation problem is to evaluate $\mathbf{G}^m = (G_1^m, G_2^m, G_3^m)$ as given by

$$G_{i}^{\mathsf{m}} = \sum_{\substack{n=1\\n\neq \mathsf{m}}}^{N} \sum_{j=1}^{3} D_{ij}(\mathbf{x}^{\mathsf{m}}, \mathbf{x}^{\mathsf{n}}, \hat{\mathbf{n}}^{\mathsf{n}}) g_{j}^{\mathsf{n}}, \quad i = 1, 2, 3, \quad \mathsf{m} = 1, \dots, N,$$
(6)

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where $\hat{\mathbf{n}}^n$ is an orientation vector at the nth source location and $\{\mathbf{g}^n = (g_1^n, g_2^n, g_3^n)\}$ are the vector source strengths. \mathbf{F}^m and \mathbf{G}^m can be thought of as velocity fields induced by point forces or surface stresses, respectively [9]. (Integrals involving S_{ij} and D_{ij} are referred to as single and double layer potentials, by analogy with the electrostatic case).

Several fast multipole methods for these kernels (or the closely related ones of linear elasticity) have been developed based essentially on expansion of the Green's function for the biharmonic equation [3,7,8,12,16]. A clever rearrangement of terms allows for the use of a total of four sets of multipole/local expansion coefficients. The cost of the method is, therefore, approximately four times that of a harmonic FMM. Recently, Wang et al. [11] have presented an efficient, parallel implementation for Stokeslet and Stresslet summations along these lines. However, none of these schemes make direct use of existing "black-box" harmonic FMMs.

Another useful approach, developed by Ying et al. [15], is the kernel independent fast multipole algorithm that can be applied to essentially any non-oscillatory kernel. This allows for straightforward "black-box" application to the Stokes equations, but at a cost of approximately six to nine scalar FMM calls (three calls with 3N sources each).

Finally, one can rewrite the Stokeslet and Stresslet summation formulas in such a way that the harmonic FMM (or any other fast electrostatic method) can be used in "black-box" fashion. This approach was taken by Wang and LeSar for dislocation dynamics [14], by Fu et al. for linear elasticity [4], and by Fu and Rodin for Stokes flow [5]. The latter formulation requires four harmonic FMM calls for Stokeslets and twelve harmonic FMM calls for Stresslets.

Here, we follow the last approach and present a new, simple and efficient decomposition of the Stokeslet and Stresslet summations into four harmonic *N*-body problems each, although the Stresslet case requires a little care (see below). It is, perhaps, worth citing three reasons for choosing to revisit this problem. First, the reformulation of the Stresslet in terms of harmonic interactions appears to be new. Second, using this approach, improvements to *any* fast algorithm for harmonic interactions, such as low-level code optimization, hardware acceleration, or parallel implementation, become available for fluid dynamic and elasticity applications. Third, the storage cost of the harmonic FMM is about half that of the biharmonic case, providing some advantage for large-scale simulations.

2. Decomposition of the stokeslet and stresslet sums

We begin by observing that the Stokeslet (3) can be written as

$$S_{ij}(\mathbf{x}, \mathbf{y}) = \left(\delta_{ij} - (x_j - y_j)\frac{\partial}{\partial x_i}\right)\frac{1}{|\mathbf{x} - \mathbf{y}|}.$$
(7)

From this, we show in Appendix A that the summation in (4) can be written as

$$F_{i}^{\mathsf{m}} = \sum_{j=1}^{3} \left[\left(\delta_{ij} - x_{j}^{\mathsf{m}} \frac{\partial}{\partial x_{i}} \right) \sum_{\substack{\mathsf{n}=1\\\mathsf{n}\neq\mathsf{m}}}^{N} \frac{f_{j}^{\mathsf{n}}}{r_{\mathsf{n}\mathsf{m}}} \right] + \frac{\partial}{\partial x_{i}} \sum_{\substack{\mathsf{n}=1\\\mathsf{n}\neq\mathsf{m}}}^{N} \frac{\mathbf{x}^{\mathsf{n}} \cdot \mathbf{f}^{\mathsf{n}}}{r_{\mathsf{n}\mathsf{m}}}, \tag{8}$$

where $\mathbf{r}_{nm} = \mathbf{x}^m - \mathbf{x}^n$ and $r_{nm} = |\mathbf{r}_{nm}|$.

That is, to compute F_i^m , i = 1, 2, 3, we need to evaluate four harmonic sums over the locations $\{\mathbf{x}^n\}$ with source strengths $\{f_j^n\}$, j = 1, 2, 3 and $\{\mathbf{x}^n \cdot \mathbf{f}^n\}$, respectively. For this, we use the FMM as described in [2], which returns both the potential and gradient due to a collection of sources. The desired results are then assembled as indicated in (8).

The Stresslet (5) can be expressed as

$$D_{ij}(\mathbf{x}, \mathbf{y}, \hat{\mathbf{n}}) = \frac{1}{6} \sum_{k=1}^{3} \left[\left(\delta_{ij} - (x_j - y_j) \frac{\partial}{\partial x_i} \right) \frac{(x_k - y_k) \hat{n}_k}{|\mathbf{x} - \mathbf{y}|^3} + \left(\delta_{ik} - (x_k - y_k) \frac{\partial}{\partial x_i} \right) \frac{(x_j - y_j) \hat{n}_k}{|\mathbf{x} - \mathbf{y}|^3} \right].$$
(9)

We leave it to the reader to verify this expression. Inserting this into the sum (6), after some algebraic manipulation (Appendix A) we get

$$G_{i}^{\mathsf{m}} = \frac{1}{6} \sum_{j=1}^{3} \left[\left(\delta_{ij} - x_{j}^{\mathsf{m}} \frac{\partial}{\partial x_{i}} \right) \sum_{\substack{\mathsf{n}=1\\\mathsf{n}\neq\mathsf{m}}}^{N} \left\{ \frac{(\mathbf{r}_{\mathsf{n}\mathsf{m}} \cdot \hat{\mathbf{n}}^{\mathsf{n}}) g_{j}^{\mathsf{n}}}{r_{\mathsf{n}\mathsf{m}}^{\mathsf{3}}} + \frac{(\mathbf{r}_{\mathsf{n}\mathsf{m}} \cdot \mathbf{g}^{\mathsf{n}}) \hat{n}_{j}^{\mathsf{n}}}{r_{\mathsf{n}\mathsf{m}}^{\mathsf{3}}} \right\} \right] \\ + \frac{1}{6} \frac{\partial}{\partial x_{i}} \sum_{\substack{\mathsf{n}=1\\\mathsf{n}\neq\mathsf{m}}}^{N} \left\{ \frac{(\mathbf{r}_{\mathsf{n}\mathsf{m}} \cdot \hat{\mathbf{n}}^{\mathsf{n}}) (\mathbf{x}^{\mathsf{n}} \cdot \mathbf{g}^{\mathsf{n}})}{r_{\mathsf{n}\mathsf{m}}^{\mathsf{3}}} + \frac{(\mathbf{r}_{\mathsf{n}\mathsf{m}} \cdot \mathbf{g}^{\mathsf{n}}) (\hat{\mathbf{n}}^{\mathsf{n}} \cdot \mathbf{x}^{\mathsf{n}})}{r_{\mathsf{n}\mathsf{m}}^{\mathsf{3}}} \right\}.$$
(10)

By comparison with (1) it is clear that to compute G_i^m , i = 1, 2, 3 requires four harmonic FMM calls, each with 2N dipole sources. For the first three calls, the orientation vectors are $\{\hat{\mathbf{n}}^n\}$ with strength $\{g_j^n\}$ and $\{\mathbf{g}^n\}$ with strength $\{\hat{n}_j^n\}$, j = 1, 2, 3. For the fourth call, the orientation vectors are $\{\hat{\mathbf{n}}^n\}$ with strength $\{\mathbf{x}^n \cdot \mathbf{g}_j^n\}$ and $\{\mathbf{g}^n\}$ with strength $\{\mathbf{x}^n \cdot \mathbf{n}^n\}$. At first glance, it might appear that the net cost would be proportional to that of 8 FMM calls, since we have doubled the number of sources. In a properly implemented FMM, however, one can have 2N sources and N targets and the net cost should be about that of 6 FMMs. We have chosen to modify the FMM code slightly to further reduce the cost as follows.

Remark 2.1. (requires some familiarity with the FMM) Two simple changes have been made. First, in the Stresslet case, when multipole expansions are formed, we incorporate the contributions from both sets of dipoles. The remaining steps of the far field calculation are the same as if there were only N sources. Second, in both the Stokeslet and Stresslet cases, we disable the nearest neighbor calculations in the first three FMM calls. In the fourth call, we use the original formulas (3) and (5) to compute nearby direct interactions only once.

The effect of these changes, as will be clear from the numerical results, is that the net cost in each case is approximately that of three FMM calls with *N* sources. We are aware that this violates one of our arguments for using harmonic FMMs, but were unable to resist.

3. Numerical results

In this section, we present some timing results for the FMM-based Stokeslet and Stresslet sums described by (4) and (6). All calculations were carried out on a laptop computer with a 1.2 GHz Pentium M processor and 500 Mb of RAM. We also present the time for an efficient implementation of direct summation, which uses only one square root evaluation to generate all nine matrix entries in (3) or (5). For the sake of comparison, we also present timings of the FMM and the direct method for simple Coulombic interactions. In the tables below, N denotes the number of sources, *Prec* denotes the number of digits of accuracy requested from the FMM, T_{FMM}^{S} denotes the time required by the FMM for Stokeslets or Stresslets, and T_{dir}^{S} denotes the direct time required for Stokeslets or Stresslets. T_{FMM}^{H} denotes the time required by the harmonic FMM for simple charge sources in the Stokeslet table and for simple dipole sources in the Stresslet table. T_{dir}^{H} denotes the time required by the direct method for the analogous summations.

To test the performance of the method on both homogeneous and inhomogeneous distributions, we carry out one set of experiments with sources distributed randomly with a uniform probability in the unit cube (*rand*), and another with sources distributed on the *surface* of a cylinder with unit radius and unit height (*cyl*). We measure the L_2 errors at N/200 sources by comparison with the direct calculation and denote the maximum of these errors for the two cases (*rand*, *cyl*) by E_{Stokes} , E_{Stress} , and E_{harmonic} . The direct timings are estimated from actual timings on N/200 sources.

There are a few things to note from the results. First, the FMM scales approximately linearly, as expected. The timings are somewhat erratic because of the fact that the adaptive FMM builds a different data structure at each precision for each source distribution. Second, the work required for Stokeslets and Stresslets is about three times greater than for the corresponding (charge or dipole) harmonic interactions. With our current implementation, the breakeven point for the FMM is about 2000 for three digits, 4000 for six digits, and 5000 for nine digits.

This is not as competitive as for the harmonic case, largely because the direct calculation for Stokeslets and Stresslets has a smaller constant associated with it. Only one square root evaluation is needed to obtain all nine matrix entries and the net time ends up being less than twice that for the harmonic case.

Table 1 Timing results for Stokeslet summation. See text for explanation

N	Prec	$T^{S}_{\rm FMM}$		$T_{\rm dir}^{\rm S}$	$T_{ m FMM}^{ m H}$		$T_{\rm dir}^{\rm H}$	Estokes	Eharmonic
		Rand	Cyl		Rand	Cyl			
4000	3	1.5	1.3	2.8	0.8	0.9	1.8	3.2×10^{-4}	3.3×10^{-4}
40,000	3	11.3	10.4	285	3.9	3.6	172	3.3×10^{-4}	5.4×10^{-4}
400,000	3	115.1	79.0	28,500	39.8	26.3	17,200	3.2×10^{-4}	1.4×10^{-3}
4000	6	2.2	2.0	2.8	0.6	1.2	1.8	1.9×10^{-7}	1.6×10^{-7}
40,000	6	23.6	21.0	285	8.1	6.7	172	1.9×10^{-7}	3.3×10^{-7}
400,000	6	327.7	261.2	28,500	108.5	83.4	17,200	1.8×10^{-7}	6.7×10^{-7}
4000	9	2.9	3.1	2.8	0.9	1.6	1.8	9.4×10^{-11}	9.2×10^{-11}
40,000	9	39.7	29.0	285	12.4	10.7	172	9.5×10^{-11}	2.5×10^{-10}
400,000	9	398.9	378.8	28,500	140.8	173.2	17,200	9.8×10^{-11}	3.1×10^{-10}

See text for explanation.

Table 2 Timing results for Stresslet summation

Ν	Prec	T^{S}_{FMM}		$T_{\rm dir}^{\rm S}$	$T_{\rm FMM}^{\rm H}$		$T_{\rm dir}^{\rm H}$	EStokes	Eharmonic
		Rand	Cyl		Rand	Cyl			
4000	3	1.5	0.9	3	0.7	0.8	2.2	3.3×10^{-3}	7.9×10^{-4}
40,000	3	14.5	12.9	300	3.9	4.2	230	6.1×10^{-4}	1.9×10^{-3}
400,000	3	134.6	102.7	30,000	47.6	30.3	23,000	1.9×10^{-3}	3.5×10^{-4}
4000	6	2.6	1.9	3	1.1	1.2	2.2	3.7×10^{-6}	5.3×10^{-7}
40,000	6	29.6	28.4	300	9.9	7.6	230	8.6×10^{-7}	1.4×10^{-6}
400,000	6	487.5	414.7	30,000	134.4	103.8	23,000	1.9×10^{-6}	2.3×10^{-7}
4000	9	3.7	3.6	3	1.5	1.7	2.2	1.8×10^{-9}	3.4×10^{-10}
40,000	9	46.6	33.4	300	15.0	15.7	230	5.5×10^{-10}	5.8×10^{-10}
400,000	9	508.0	522.2	30,000	173.7	146.7	23,000	1.2×10^{-9}	7.7×10^{-11}

See text for explanation.

In any event, with 400,000 sources at six digits of accuracy, speedup factors of 100 and 70 are obtained for Stokeslets and Stresslets, respectively. More generally, the time for Stokeslet summation is about 30% faster than for Stresslet summation. The reasons for this are somewhat complex and involve detailed aspects of the FMM implementation. We believe this additional cost could be eliminated with more detailed changes to the code. We have chosen not to make these changes in order to hold to our original aim, which was to use black box harmonic FMMs. We have already violated that notion (Remark 2.1), because the change was so minor. As a matter of full disclosure, using unmodified, black box FMMs for 40,000 Stokeslets at 6 digits of accuracy requires 31.8 s, instead of the 23.6 s indicated in Table 1. Not surprisingly, this is very close to four times the cost of the harmonic FMM. Using black box FMMs for 40,000 Stresslets at 6 digits of accuracy requires about 60 s instead of the 29.6 s indicated in Table 2. As expected, this is very close to six times the cost of the corresponding harmonic FMM (see paragraph above Remark 2.1).

4. Conclusions

In this paper, we have presented a fast multipole method (FMM) for Stokeslet and Stresslet calculations, based on the use of the harmonic FMM. Each of the Stresslet and Stokeslet summations requires four calls to such an FMM, which has been trivially modified so that the net cost scales like three harmonic interactions. A feature of our approach is that additional improvements to any fast algorithm for harmonic interactions, from code optimization to specialized hardware, become immediately available for Stokesian particle dynamics and integral equation methods in fluid dynamics.

The FMM requirements for linear elasticity are slightly different than those presented here. While the kernel for the single layer potential is essentially the Stokeslet, the kernel for the double layer potential differs somewhat from the fluid Stresslet. Nevertheless, as already shown in [4,14], it is possible to develop a fast algorithm using only harmonic FMMs. Analytic manipulations like those presented in the Appendix can reduce the total number of harmonic *N*-body problems required and will be reported at a later date.

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Appendix A.

From the formula for the Stokeslet in (7), we can write

$$\sum_{j=1}^{3} S_{ij}(\mathbf{x}, \mathbf{y}) f_{j} = \sum_{j=1}^{3} \left(\delta_{ij} - x_{j} \frac{\partial}{\partial x_{i}} \right) \frac{f_{j}}{|\mathbf{x} - \mathbf{y}|} + \sum_{j=1}^{3} y_{j} \frac{\partial}{\partial x_{i}} \frac{f_{j}}{|\mathbf{x} - \mathbf{y}|}$$
$$= \sum_{j=1}^{3} \left[\left(\delta_{ij} - x_{j} \frac{\partial}{\partial x_{i}} \right) \frac{f_{j}}{|\mathbf{x} - \mathbf{y}|} \right] + \frac{\partial}{\partial x_{i}} \frac{\mathbf{y} \cdot \mathbf{f}}{|\mathbf{x} - \mathbf{y}|}. \tag{11}$$

Inserting this into (4), we get

$$F_{i}^{\mathsf{m}} = \sum_{\substack{\mathsf{n}=1\\\mathsf{n}\neq\mathsf{m}}}^{N} \sum_{j=1}^{3} S_{ij}(\mathbf{x}^{\mathsf{m}}, \mathbf{x}^{\mathsf{n}}) f_{j}^{\mathsf{n}} = \sum_{\substack{\mathsf{n}=1\\\mathsf{n}\neq\mathsf{m}}}^{N} \left[\sum_{j=1}^{3} \left[\left(\delta_{ij} - x_{j}^{\mathsf{m}} \frac{\partial}{\partial x_{i}} \right) \frac{f_{j}^{\mathsf{n}}}{r_{\mathsf{n}\mathsf{m}}} \right] + \frac{\partial}{\partial x_{i}} \frac{\mathbf{x}^{\mathsf{n}} \cdot \mathbf{f}^{\mathsf{n}}}{r_{\mathsf{n}\mathsf{m}}} \right],$$
(12)

where $r_{nm} = |\mathbf{x}^m - \mathbf{x}^n|$. Interchanging the order of summation, we obtain the result in (8).

Using the expression for the Stresslet given in (9), we get

$$\begin{split} \sum_{j=1}^{3} D_{ij}(\mathbf{x}, \mathbf{y}, \hat{\mathbf{n}}) g_{j} &= \frac{1}{6} \sum_{j=1}^{3} \sum_{k=1}^{3} \left[\left(\delta_{ij} - x_{j} \frac{\partial}{\partial x_{i}} \right) \frac{(x_{k} - y_{k}) \hat{n}_{k} g_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} + \left(\delta_{ik} - x_{k} \frac{\partial}{\partial x_{i}} \right) \frac{(x_{j} - y_{j}) \hat{n}_{k} g_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} \right. \\ &\quad + \frac{\partial}{\partial x_{i}} \frac{(x_{k} - y_{k}) \hat{n}_{k} y_{j} g_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} + \frac{\partial}{\partial x_{i}} \frac{(x_{j} - y_{j}) \hat{n}_{k} y_{k} g_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} \right] \\ &= \frac{1}{6} \sum_{j=1}^{3} \sum_{k=1}^{3} \left[\left(\delta_{ij} - x_{j} \frac{\partial}{\partial x_{i}} \right) \left\{ \frac{(x_{k} - y_{k}) \hat{n}_{k} g_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} + \frac{(x_{k} - y_{k}) \hat{n}_{j} g_{k}}{|\mathbf{x} - \mathbf{y}|^{3}} \right\} \\ &\quad + \frac{\partial}{\partial x_{i}} \left\{ \frac{(x_{k} - y_{k}) \hat{n}_{k} y_{j} g_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} + \frac{(x_{k} - y_{k}) g_{k} \hat{n}_{j} y_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} \right\} \right], \end{split}$$

where we have swapped the dummy indices j and k in the second and fourth terms after the second equality sign. We can now carry out the sum over k, and write

$$\begin{split} \sum_{j=1}^{3} D_{ij}(\mathbf{x}, \mathbf{y}, \hat{\mathbf{n}}) g_{j} &= \frac{1}{6} \sum_{j=1}^{3} \left(\delta_{ij} - x_{j} \frac{\partial}{\partial x_{i}} \right) \left\{ \frac{\left((\mathbf{x} - \mathbf{y}) \cdot \hat{\mathbf{n}} \right) g_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} + \frac{\left((\mathbf{x} - \mathbf{y}) \cdot \mathbf{g} \right) \hat{n}_{j}}{|\mathbf{x} - \mathbf{y}|^{3}} \right\} \\ &+ \frac{1}{6} \frac{\partial}{\partial x_{i}} \left\{ \frac{\left((\mathbf{x} - \mathbf{y}) \cdot \hat{\mathbf{n}} \right) (\mathbf{y} \cdot \mathbf{g})}{|\mathbf{x} - \mathbf{y}|^{3}} + \frac{\left((\mathbf{x} - \mathbf{y}) \cdot \mathbf{g} \right) (\hat{\mathbf{n}} \cdot \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^{3}} \right\}. \end{split}$$

Inserting this into the sum in (6), we get

$$G_{i}^{\mathsf{m}} = \frac{1}{6} \sum_{\substack{n=1\\n\neq m}}^{N} \sum_{j=1}^{3} \left(\delta_{ij} - x_{j}^{\mathsf{m}} \frac{\partial}{\partial x_{i}} \right) \left\{ \frac{(\mathbf{r}_{\mathsf{nm}} \cdot \hat{\mathbf{n}}^{\mathsf{n}})g_{j}^{\mathsf{n}}}{r_{\mathsf{nm}}^{\mathsf{3}}} + \frac{(\mathbf{r}_{\mathsf{nm}} \cdot \mathbf{g}^{\mathsf{n}})\hat{n}_{j}}{r_{\mathsf{nm}}^{\mathsf{3}}} \right\} + \frac{1}{6} \sum_{\substack{n=1\\n\neq m}}^{N} \frac{\partial}{\partial x_{i}} \left\{ \frac{(\mathbf{r}_{\mathsf{nm}} \cdot \hat{\mathbf{n}}^{\mathsf{n}})(\mathbf{x}^{\mathsf{n}} \cdot \mathbf{g}^{\mathsf{n}})}{r_{\mathsf{nm}}^{\mathsf{3}}} + \frac{(\mathbf{r}_{\mathsf{nm}} \cdot \mathbf{g}^{\mathsf{n}})(\hat{\mathbf{n}}^{\mathsf{n}} \cdot \mathbf{x}^{\mathsf{n}})}{r_{\mathsf{nm}}^{\mathsf{3}}} \right\},$$
(13)

where we have introduced the notation $\mathbf{r}_{nm} = \mathbf{x}^m - \mathbf{x}^n$, and $r_{nm} = |\mathbf{r}_{nm}|$. Moving in the sum over n, we obtain the result in (10).

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