Efficient Evaluation of Matrix Elements between Distant Basis Functions in LIBSCUFF

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Contents

1 Overview

2 Cartesian Multipole Technique

$$G_{\mu\nu}(\mathbf{r}) = G_{\mu\nu}(\mathbf{r}_0) + (\mathbf{r}-\mathbf{r}_0)_\rho G_{\mu\nu\rho}(\mathbf{r}_0) + \frac{1}{2}(\mathbf{r}-\mathbf{r}_0)_\rho(\mathbf{r}-\mathbf{r}_0)_\sigma G_{\mu\nu\rho\sigma}(\mathbf{r}_0) + \cdots$$

$$\begin{aligned}
&\int\int f_{m\mu}(\mathbf{x}) G_{\mu\nu}(\mathbf{x}-\mathbf{x}') f_{n\nu}(\mathbf{x}') d\mathbf{x} d d\mathbf{x}' \\
&= G^0_{\mu\nu} \underbrace{\left[\int f_{m\mu}(\mathbf{x})\, d\mathbf{x}\right]}_{\mathcal{M}_{m\mu}} \underbrace{\left[\int f_{n\nu}(\mathbf{x}')\, d\mathbf{x}'\right]}_{\mathcal{M}_{n\nu}} \\
&+ G^0_{\mu\nu\rho}\left\{ \underbrace{\left[\int (\mathbf{x}-\mathbf{x}_0)_\rho f_{m\mu}(\mathbf{x})\, d\mathbf{x}\right]}_{\mathcal{M}_{m\mu\rho}} \underbrace{\left[\int f_{n\nu}(\mathbf{x}')\, d\mathbf{x}'\right]}_{\mathcal{M}_{n\nu}} - \underbrace{\left[\int f_{m\mu}(\mathbf{x})\, d\mathbf{x}\right]}_{\mathcal{M}_{m\mu}} \underbrace{\left[\int (\mathbf{x}'-\mathbf{x}'_0)_\rho f_{n\nu}(\mathbf{x}')\, d\mathbf{x}'\right]}_{\mathcal{M}_{n\nu\rho}} \right\} \\
&+ \cdots
\end{aligned}$$

Multipole moments of RWG basis functions

$$\begin{aligned}
\mathcal{M}_{m\mu} &= \frac{l_m}{3}\Big(\mathbf{Q}^-_m - \mathbf{Q}^+_m\Big)_\mu \\
\mathcal{M}_{m\mu\rho} &= \frac{l_m}{12}\Big[\mathbf{A}^-_\mu \mathbf{A}^-_\rho - \mathbf{A}^+_\mu \mathbf{A}^+_\rho\Big] - \frac{1}{8}\Big[\mathbf{B}_\mu \mathcal{M}_{m\rho} + \mathcal{M}_{m\mu}\mathbf{B}_\rho\Big]
\end{aligned}$$

Cartesian Components of Dyadic Green's functions

$$\begin{aligned}
G_{\mu\nu}(\mathbf{r}) &= \left[P_1(ikr)\delta_{\mu\nu} + P_2(ikr)\frac{r_\mu r_\nu}{r^2}\right]\Phi(r) \\
C_{\mu\nu}(\mathbf{r}) &= ikP_3(ikr)\Phi(r)\varepsilon_{\mu\nu\rho}r_\rho
\end{aligned}$$

$$\begin{aligned}
\Phi(r) &= \frac{e^{ikr}}{4\pi(ik)^2 r^3} \\
P_1(x) &= 1 - x - x^2 \\
P_2(x) &= -3 + 3x - x^2 \\
P_3(x) &= -1 + x
\end{aligned}$$

First derivatives

$$\begin{aligned}
G_{\mu\nu\rho}(\mathbf{r}) &= \frac{d}{dr_\rho}G_{\mu\nu}(\mathbf{r}) \qquad\qquad = \left[P_1(ikr)\delta_{\mu\nu} + P_2(ikr)\frac{r_\mu r_\nu}{r^2}\right]\Phi(r) \\
C_{\mu\nu}(\mathbf{r}) &= ikP_3(ikr)\Phi(r)\varepsilon_{\mu\nu\rho}r_\rho
\end{aligned}$$

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\begin{aligned}
\Phi(r) &= \frac{e^{ikr}}{4\pi(ik)^2 r^3} \\
P_1(x) &= 1 - x - x^2 \\
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\end{aligned}
$$