MULTIPOLES FROM REAL SPACE QUADRATURE

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WHAT IS A MULTIPOLe EXPANSION?

A coefficient.

\[ f(x) = f(0) + xf'(0) + \frac{x^2}{2} f''(0) + \ldots \]

\[ \Phi(r) = \sum_{n=0} \frac{((r - r_0) \cdot \partial_s)^n}{n!} \frac{1}{|s|} \bigg|_{s=r_0} \]
FAR-FIELD INTERACTION $E$

- Potential function expansion
- Transferable, Polarizable FFs
- Fast multipole method, $O(N)$

\[
V_{AB}^{es} = M_A \cdot T_{AB} \cdot \tilde{M}_B
\]

\[
M = \begin{pmatrix} q \\ \vec{\mu} \\ Q \end{pmatrix}
\]

\[
T = \begin{bmatrix} r^{-1} & \partial r^{-1} & \partial^{(2)} r^{-1} \\ \partial r^{-1} & \partial^{(2)} r^{-1} & \partial^{(3)} r^{-1} \\ \partial^{(2)} r^{-1} & \partial^{(3)} r^{-1} & \partial^{(4)} r^{-1} \end{bmatrix}
\]

Jacobson, Williams, Herbert, JCP 130, 2009.
BUT IT’S NOT SO SIMPLE?

Spherical multipoles are efficient, yet unintelligible.

\[ \partial_{\alpha\beta\gamma\delta}^{(4)} \]

Cartesian: \(3^4 = 81\) component tensor!

\[
M_{lm} = \sum q_i |r_p|^l C_{lm}(\hat{r}_p)
\]

\[
V_{l,k} = \left(\frac{2l + 2k}{2l}\right)^{1/2} R^{-l-k-1} \sum_{m=-l-k}^{l+k} (-1)^m C_{l+k,-m}(\hat{R}) [M_A^{(l)} \otimes M_B^{(k)}]_{l+k,m}
\]

\[
[M_A^{(l)} \otimes M_B^{(k)}]_{l+k,m} = \sum_{n=-l}^{l} \sum_{j=-k}^{k} M_A^{(l)} M_B^{(k)} \langle l, n; k, j | l + k, m \rangle
\]

THE REAL PROBLEM

\[ \frac{1}{|x - y|} = e^{-y \cdot \partial} \frac{1}{|x|} = \sum_{l=0}^{l} \frac{|y|^l}{|x|^{l+1}} P_n(\hat{x} \cdot \hat{y}) \]

\[ = \sum_{l=0}^{l} \sum_{m=-l}^{l} O_{l,m}(x)M_{l,m}(y) \]

\[ O_{l,m}(x) = |x|^l (l + |m|)! P_{l,m}(\cos \theta_x) e^{-im\phi_x} \]

\[ M_{l,m}(x) = |x|^{-l-1} (l - |m|)!^{-1} P_{l,m}(\cos \theta_x) e^{im\phi_x} \]

One step too far!

White and Head-Gordon, JCP 101, 1994.
THE REAL PROBLEM

\[
\frac{1}{|x - y|} = e^{-y \cdot \partial} \frac{1}{|x|} = \sum_{l=0} \frac{|y|^l}{|x|^{l+1}} P_n(\hat{x} \cdot \hat{y}) = \sum_{l=0} \frac{|y|^l}{|x|^{l+1}n!} \hat{x}^{(n)} (n) \hat{y}^{(n)}
\]

\[
\partial^{(n)} |r|^{-1} = (-1)^n |r|^{-2n-1} \mathcal{T}_n r^{(n)}
\]

One step too far!

$(-y \cdot \partial)^n |x|^{-1} / n! = L_n(y, x)$  \hspace{1cm} \textbf{directional derivative}

$= \int_S L_n(y, \hat{r}) K(\hat{r}, x) \, d^2\hat{r}$  \hspace{1cm} \textbf{spherical projection}

\textbf{BACK TO THE DRAWING BOARD.}

QUADRATURE

- Optimal number of points ($p^2$)
- Physical interpretation = surface charge distribution

$$\int_S f(y, \hat{r}) \sigma(\hat{r}) \, d^2\hat{r} = \sum_i (w_i \sigma(\hat{r}_i)) f(y, \hat{r}_i)$$
INNER EXPANSION

\[ \sigma_i(\hat{r}) = \int K(\hat{r}, x) \rho(x) \, d^3 x \]

OUTER EXPANSION

\[ \sigma_o(\hat{r}) = \int \rho(y) K(y, \hat{r}) \, d^3 y \]

• Getting in is easy
INNER EXPANSION

\[
\Phi(y) = \int_S \sum_n L_n(y, \hat{r}) \sigma_i(\hat{r}) \, d^2\hat{r}
\]

\[
\approx \frac{q_i}{|y - \hat{r}_i|} \quad \text{(may require scaling $S$)}
\]

OUTER EXPANSION

\[
\Phi(x) = \int_S \sigma_o(\hat{r}) \sum_n L_n(\hat{r}, x) \, d^2\hat{r}
\]

\[
\approx \frac{q_i}{|x - \hat{r}_i|}
\]

• Getting out is **even easier**!
The error of the inner expansion shows much more variation as a function of the cosine with respect to the shift direction, since the distance between the rightmost point of original evaluation and the shifted version.

For the inner expansion, the source points were scaled down for each shift to maintain contact with the rightmost face of the source distribution is shifted to the right by 0.1, 0.2, 0.3, and 0.4, with weights had nearly identical error (not shown).

For comparison, the simple summation of quadrature-based representation gives highly accurate point charges that simultaneously represent all multipoles. Practically, this solves the problem of placing accurate point charges that simultaneously represent all multipoles. This is also the reason for the symmetry of the shifting formulas – the weights mimic all multipolar moments up to arbitrary order.

Table 1: Boundary integrals over a source distribution on a spherical surface.

Rogers (submitted), 2014.
FUN WITH MULTipoLES

\[
v(x) \equiv -\partial \Phi(x)
\]
\[
0 = \partial^2 \Phi(x)
\]
\[
n \cdot v(x) = v_0(x), x \in \partial \Omega
\]

Figure 4: Multipole representation of potential flow for three spheres in the \( z = 0 \) plane (upper panel, \( p = 8 \)). Color indicates the potential field. The flow velocity was rendered using line integral convolution. The lower panel shows the surface-averaged boundary error divided into contributions from the larger and smaller spheres.
WORK WITH MULTIPOLES

CONCLUSIONS

• Spherical harmonics considered harmful
  • May have convergence issues!
• Real-space Quadrature
  • Basis vectors are real
  • Weights are charges
  • Approx. power and dimension identical
  • Symmetry is apparent
  • Shifting functions are identical to initial fitting!
    Rogers (submitted), 2014.

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