MATHEMATICAL DERIVATION OF AN ALTERNATIVE FAST MULTIPOLE METHOD.

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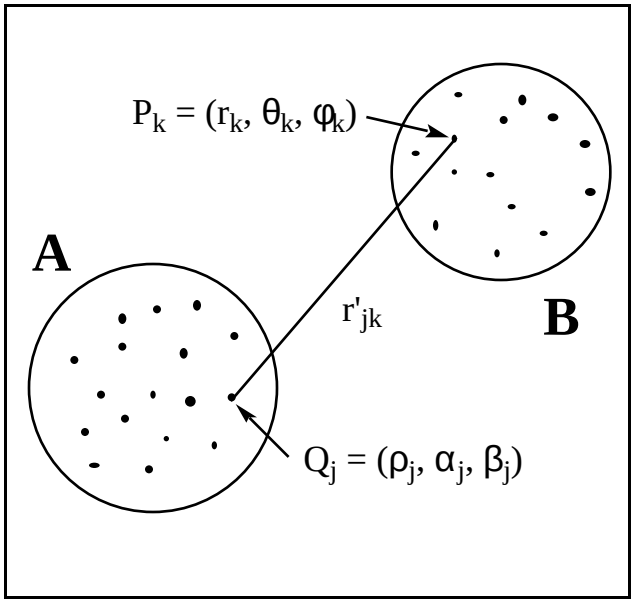
Many problems in modern chemistry involve the computation of electrostatic interactions between large numbers of distant atoms and molecules. Due to the $O(N^2)$ nature of the N-body problem, the computational requirements quickly become overwhelming. Numerical techniques designed to deal with large N generally compute some kind of "average" for the particles in groups A and B. These "averages" are then used to estimate the potential between distributions A and B. One method that has been successful is the Fast Multipole Method (FMM). The basic form of the FMM formula is given in equation 1. Equation 1 leads naturally to the question: does there exist an expression for the potential of the form shown in equation 2-1?



$$\sum_{m=0}^{\infty} \sum_{B} B_m(P_k) \sum_{A} A_m(Q_j) \qquad \text{(equation 1)}$$

$$\sum_{m=0}^{\infty} \left(\sum_{B} B_m(P_k) \right) \left(\sum_{A} A_m(Q_j) \right) \qquad \text{(equation 2-1)}$$

$$\sum_{m=0}^{\infty} \left(\int_{B} B_m(P_k) \right) \left(\int_{A} A_m(Q_j) \right) \qquad \text{(equation 2-2)}$$

Since chemistry deals with continuous charge distributions a more appropriate form might be equation 2-2. Equation 2 offers the advantage that the summations over A and B are independent of each other. This property should allow for a more efficient implementation of a fast multipole algorithm. In this presentation, the mathematical derivation will be presented for a fast multipole algorithm that takes the desired form of equation 2-2.