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Foundations of Algorithms and Computational Techniques in Systems Biology
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known

$$\underbrace{\frac{\partial \psi_p(\vec{x}_{c_i})}{\partial n}}_{\text{Panel Charge Potential}} - \frac{\sigma_i}{\frac{\epsilon_{in}}{4\pi\epsilon_r}(1-\epsilon_r)} = -\underbrace{\frac{\partial \psi_A(\vec{x}_{c_i})}{\partial n}}_{\text{Atomic Charge Potential}}$$

Dense

$$P\vec{\sigma}_p = \vec{\psi}_A$$

Iterate: Guess at $\vec{\sigma}_P^0$

Calculate $\vec{\psi}_A - P\vec{\sigma}_P^0 = \text{Residual}$

$\vec{\sigma}_P^1 = f(\text{Residual})$

~~Matrix Vector Product~~ ← N potential derivatives from N charges using Multipole $O(N)$

$$\begin{array}{r} \\ \text{Row } \vec{x}_{c_1} \rightarrow \\ \\ j^{th} \\ \\ \\ \text{Row } \vec{x}_{c_N} \rightarrow \end{array}
\overbrace{\begin{bmatrix} & i^{th} & \\ & & \\ & \frac{\partial}{\partial n_j}\int_{\text{Panel } i} \frac{1}{|x' - x_{c_j}|}\, dS' & \\ & & \\ & \text{DENSE MATRIX (Every element is nonzero)} & \end{bmatrix}}^{\psi_P}
\begin{bmatrix} \sigma_1 \\ \vdots \\ \sigma_i \\ \vdots \\ \sigma_N \end{bmatrix}
= - \overbrace{\begin{bmatrix} \frac{\partial}{\partial n_1}\sum \frac{q_i}{\epsilon_{in}|\vec{x}_{c_1} - \vec{x}_i|} \\ \vdots \\ \frac{\partial}{\partial n_j}\sum \frac{q_i}{\epsilon_{in}|\vec{x}_{c_j} - \vec{x}_i|} \\ \vdots \\ \frac{\partial}{\partial n_N}\sum \frac{q_i}{\epsilon_{in}|\vec{x}_{c_N} - \vec{x}_i|} \end{bmatrix}}^{\psi_A}$$

Diagonal terms: $+ \frac{1}{\frac{\epsilon_{in}}{4\pi\epsilon_r}(1-\epsilon_r)}$