Boundary conditions in multipole techniques

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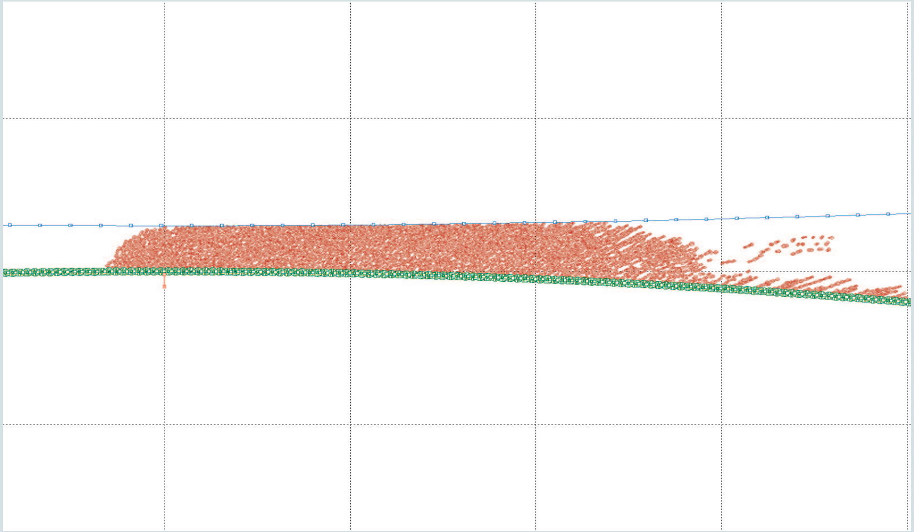
1. Introduction



Molecular dynamics: follow the trajectories of N particles by Newton's second law:

$$m_i \frac{d^2 x_i}{dt^2} = -\nabla \Phi_i, \qquad i = 1, ..., N.$$

2. Multipole method

Fast multipole method

N charged particles lead to N^2 pairwise interactions from Coulomb's law, i.e.

$$\Phi_{ij} = \frac{q_j}{4\pi\varepsilon_0 \|\mathbf{x}_i - \mathbf{x}_j\|}, \qquad i, j = 1, \ldots, N.$$

Taylor series multipole expansions

$$f(z) = \sum_{n=0}^{\infty} c_n (z-a)^n, \qquad c_n = \frac{f^{(n)}(a)}{n!},$$

in particular

$$\frac{1}{\|\mathbf{x} - \mathbf{x}_0\|} = \frac{1}{|z - z_0|} = \frac{1}{|z|} \cdot \frac{1}{|1 - z_0/z|} = \frac{1}{|z|} \Big| \sum_{n=0}^{\infty} \left(\frac{z_0}{z}\right)^n \Big|,$$

lead to an algorithm requiring an amount of work proportional to N to evaluate all interactions.

Multipole method in physics

Consider the electrostatic problem:

$$\nabla^2 V(\mathbf{x}) = -\frac{\rho(\mathbf{x})}{\varepsilon_0} = \frac{1}{\varepsilon_0}\int \rho(\mathbf{y})\left(-\delta(\mathbf{x}-\mathbf{y})\right) d\tau_{\mathbf{y}}.$$

Its formal solution is:

$$V(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0}\int \frac{\rho(\mathbf{y})}{\|\mathbf{x}-\mathbf{y}\|} d\tau_{\mathbf{y}}.$$

Since

$$\|\mathbf{x}-\mathbf{y}\|^2 = \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 - 2\left(\mathbf{x},\mathbf{y}\right) = \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 - 2\|\mathbf{x}\|\,\|\mathbf{y}\|\cos\theta,$$

we have that

$$\frac{1}{\|\mathbf{x}-\mathbf{y}\|} = \frac{1}{\|\mathbf{x}\|}\frac{1}{\left(1 - 2\frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}\cos\theta + \left(\frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}\right)^2\right)^{1/2}} = \frac{1}{\|\mathbf{x}\|}\sum_{n=0}^{\infty} P_n(\cos\theta)\left(\frac{\|\mathbf{y}\|}{\|\mathbf{x}\|}\right)^n$$

This leads to

$$
\begin{aligned}
V(\mathbf{x}) &= \frac{1}{4\pi\varepsilon_0} \int \frac{\rho(\mathbf{y})}{\|\mathbf{x}\|} \sum_{n=0}^{\infty} P_n(\cos\theta) \left(\frac{\|\mathbf{y}\|}{\|\mathbf{x}\|} \right)^n d\tau_{\mathbf{y}} \\
&= \frac{1}{4\pi\varepsilon_0 \|\mathbf{x}\|} \left(\int \rho(\mathbf{y}) d\tau_{\mathbf{y}} + \frac{1}{\|\mathbf{x}\|} \left(\frac{\mathbf{x}}{\|\mathbf{x}\|}, \int \rho(\mathbf{y}) \mathbf{y} d\tau_{\mathbf{y}} \right) + \ldots \right) \\
&= \frac{1}{4\pi\varepsilon_0 \|\mathbf{x}\|} \left(Q + \frac{1}{|\mathbf{x}||} \left(\frac{\mathbf{x}}{\|\mathbf{x}\|}, \mathbf{p} \right) + \ldots \right),
\end{aligned}
$$

Q: total charge,
$\mathbf{p}$: electric dipole moment.

Conclusion

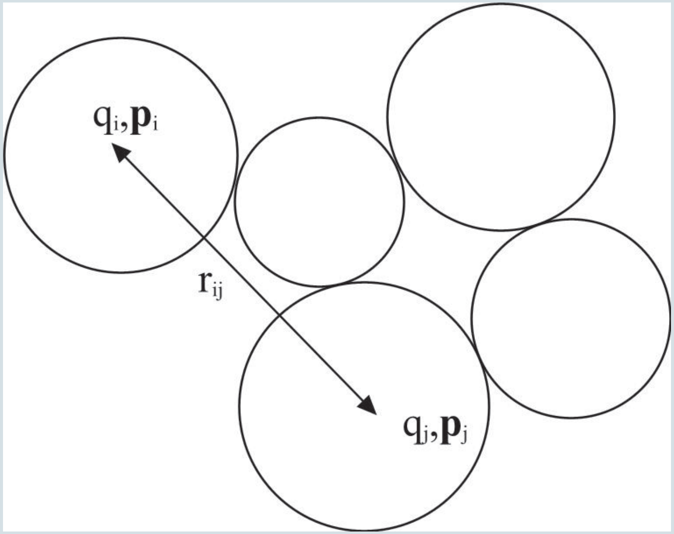
In physics, the multipole method is an integrated version of the fast multi-pole method.

3. Conducting agglomerates

Theory

Based on "Polarizability of conducting and dielectric agglomerates: theory and experiment" by R.C. Brown and M.A. Hemingway in Journal of Electrostatics 53 (2001) 235-254.

Consider a conducting agglomerate in an external electric field $\mathbf{E}_0$:



The response of a conductor to an external electric field will be such that the entire agglomerate has a constant electric potential.

$$V_{ijq} = \frac{q_j}{4\pi\varepsilon_0 r_{ij}}, \qquad \mathbf{E}_{ijq} = -\nabla V_{ijq},$$

$$V_{ijp} = \frac{(\mathbf{p}_j, \mathbf{r}_{ij})}{4\pi\varepsilon_0 r_{ij}^3}, \qquad \mathbf{E}_{ijp} = -\nabla V_{ijp}.$$

This yields

$$V_i = \sum_{j\neq i} \left(V_{ijq} + V_{ijp} - \mathbf{E}_0 \cdot \mathbf{r}_i\right), \qquad \mathbf{E}_i = \sum_{j\neq i} \left(-\nabla V_{ijq} - \nabla V_{ijp}\right) + \mathbf{E}_0.$$

Furthermore, the dipole moment $\mathbf{p}$, developed by a conducting sphere of radius R in a uniform electric field $\mathbf{E}_0$ is given by

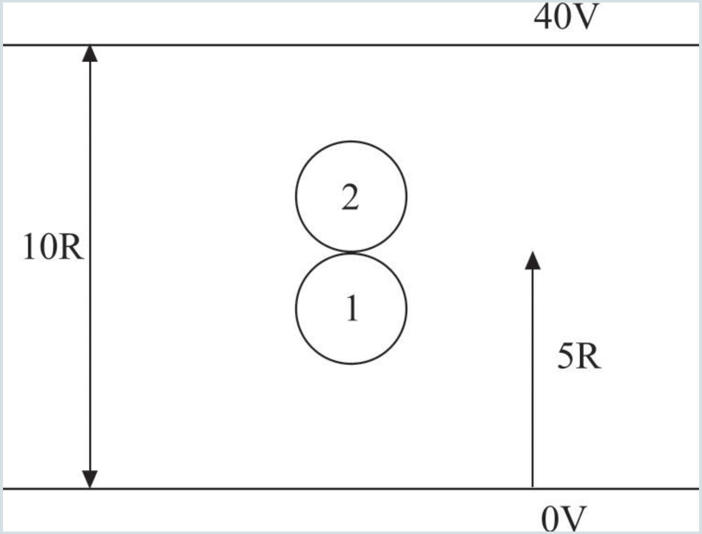
$$\mathbf{p} = 4\pi\varepsilon_0 R^3 \mathbf{E}_0.$$

Imposed conditions:

$$V_i = V, \qquad \mathbf{p}_i = 4\pi\varepsilon_0 R_i^3 \mathbf{E}_i, \qquad \sum_i q_i = 0.$$

Unknown: q_i, $\mathbf{p}_i$, V, i.e. 4N+1.
Linear equations: 4N+1.

An example



In this case: $\mathbf{E}_0 = -40/(10R)\mathbf{e}_y$ and $r_{12} = r_{21} = 2R$. This gives

$$V_1 = 16 + \frac{q_2}{8\pi\varepsilon_0 R} = V, \qquad V_2 = 24 + \frac{q_1}{8\pi\varepsilon_0 R} = V, \qquad q_1 + q_2 = 0,$$

with solution

$$q_1 = -32\pi\varepsilon_0 R, \qquad q_2 = +32\pi\varepsilon_0 R, \qquad V = 20.$$

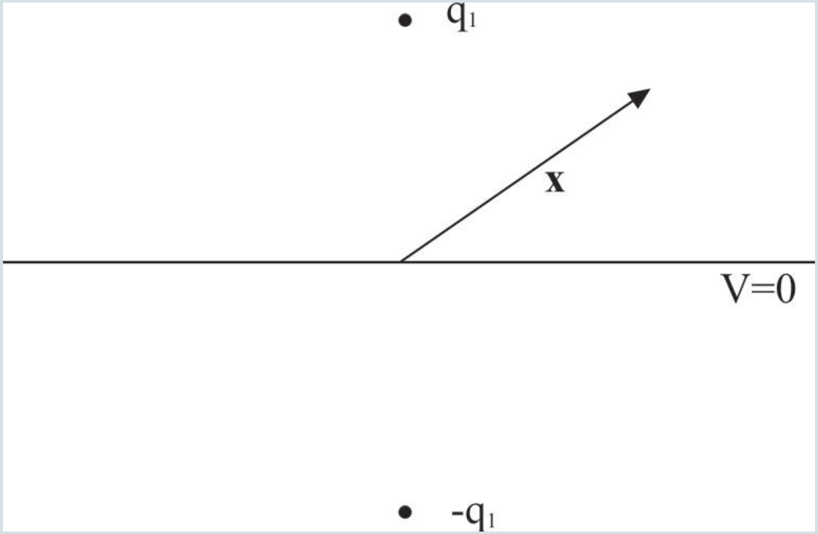
Corrections

- Replace the condition $V_i = V$ by $\frac{1}{4\pi R_i^2}\oint_{\partial B(\mathbf{x}_i, R_i)} V_i^{new} d\sigma = V$, where $V_i^{new} = V_i + V_{iiq} + V_{iip}$.
- Use higher order terms (quadrupole, octapole, et cetera) in the multipole expansion to model the conducting contact better. What happens at the boundary $\|\mathbf{x}\| = R$ of a conducting sphere ?

$$\begin{aligned}
V(\mathbf{x}) &= \frac{1}{4\pi\varepsilon_0\|x\|}\sum_{n=0}^{\infty}\int \sigma\delta(\|\mathbf{y}\| - R)P_n(\cos\theta)\left(\frac{\|\mathbf{y}\|}{R}\right)^n d\tau \\
&= \frac{\sigma}{4\pi\varepsilon_0 R}\sum_{n=0}^{\infty} 2\pi R^2 \int_0^{\pi} P_n(\cos\theta)\sin\theta d\theta \\
&= \frac{\sigma R}{2\varepsilon_0}\sum_{n=0}^{\infty}\int_{-1}^{1} P_n(z)\cdot 1 dz \\
&= \frac{\sigma R}{2\varepsilon_0}\sum_{n=0}^{\infty}\frac{2}{2n+1}\delta_{n0} = \frac{\sigma R}{\varepsilon_0}
\end{aligned}$$

Boundary conditions

First a simple case: 1 point charge q_1 opposite to a grounded plate.



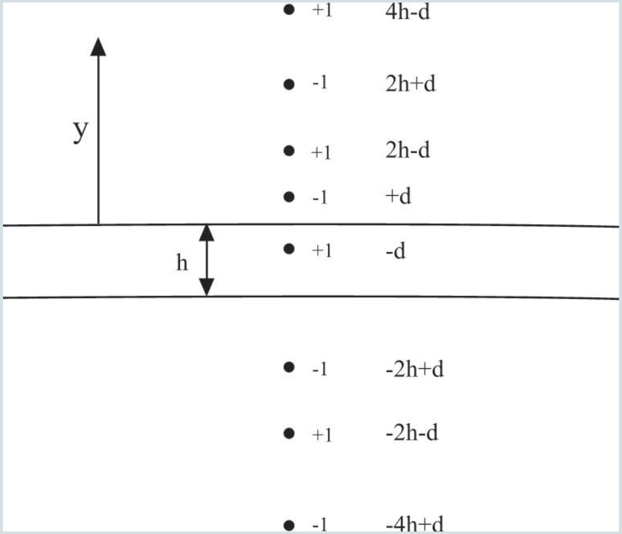
Then:

$$V(\mathbf{x}) \neq V_{q_1}(\mathbf{x}) = \frac{q_1}{4\pi\varepsilon_0 \|\mathbf{x} - \mathbf{x}_1\|},$$

$$V(\mathbf{x}) = V_{q_1}(\mathbf{x}) + V_{q_2}(\mathbf{x}) = \frac{q_1}{4\pi\varepsilon_0}\left(\frac{1}{\|\mathbf{x} - \mathbf{x}_1\|} - \frac{1}{\|\mathbf{x} - \mathbf{x}_2\|}\right).$$

4. Image charges

Consider a point charge between two grounded plates.

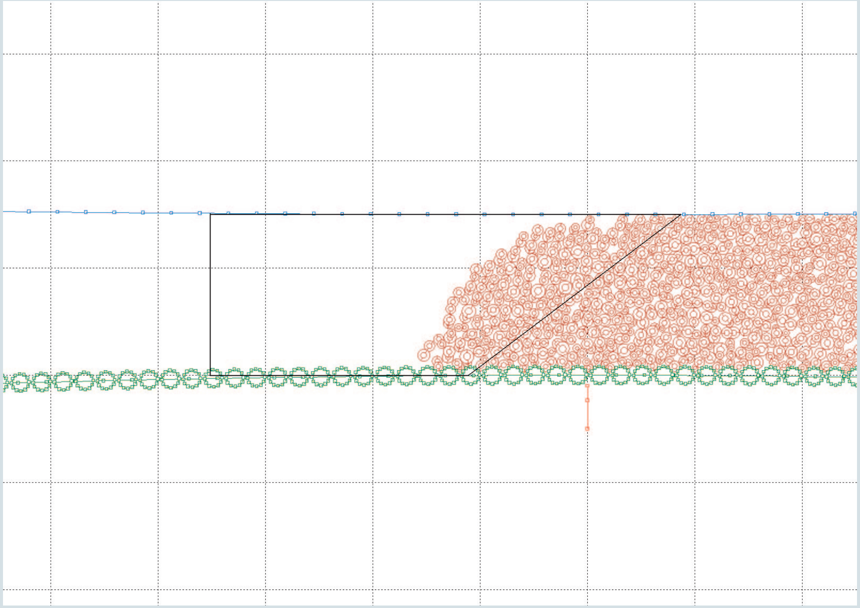


Positive charges: $-d, 2h-d, -2h-d, 4h-d, -4h-d, \ldots,$
$-d+2kh,\ k \in \mathbb{Z}$.
Negative charges: $d, -2h+d, 2h+d, -4h+d, 4h+d, \ldots,$
$d+2kh,\ k \in \mathbb{Z}$.

This leads to

$$V(\mathbf{x}) = \frac{1}{4\pi\varepsilon_0}\sum_{k\in\mathbb{Z}}\left(\frac{1}{\|\mathbf{x}-(-d+2kh)\mathbf{e}_y\|} - \frac{1}{\|\mathbf{x}-(d+2kh)\mathbf{e}_y\|}\right).$$

In reality:



This leads to millions of calculations.

5. Conclusions

- Multipole methods are often used by physicists and engineers, and give general insight into the problem.
- For a multipole expansion the correct fundamental solution (function of Green) is required.
- The potential cannot in general be calculated from merely the point charges.
- The calculation of image charges converges very slowly for real life problems. This makes the Fast Multipole Method very slow.