Analytic description of the particle-particle, particle-mesh method

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1 Coulomb force

Consider a collection of N_p point particles with positions $x = \{x_1, x_2, \ldots, x_{N_p}\}$ and charges $q = \{q_1, q_2, \ldots, q_{N_p}\}$; each $x_j \in \mathbb{R}^3$ and $q_j \in \mathbb{R}$. The Coulomb force on particle i due to the others is

$$F_C^i = q_i E_C(x_i) \tag{1}$$

$$= -q_i \left(\nabla(-\Delta)^{-1} \frac{1}{\epsilon_0} \sum_{j=1, j \neq i}^{N_p} q_j \delta_{x_j} \right)(x_i) \tag{2}$$

$$= \frac{q_i}{4\pi\epsilon_0} \sum_{j=1, j \neq i}^{N_p} \frac{q_j}{|x_i - x_j|^3}(x_i - x_j), \tag{3}$$

where δ_x is the Dirac-delta distribution centered at x. The total cost to compute the Coulomb force on every particle due to all the others is $\mathcal{O}(N_p^2)$, which is prohibitively large for sufficiently large N_p. A cheaper alternative to compute the electrostatic force on particle i is the PIC approach.

2 Particle-in-cell (PIC) approach

Let $S_a : \mathbb{R}^3 \to \mathbb{R}$ be a smooth function with fixed compact support of diameter $a > 0$ that integrates to 1, and define the smoothing operator $\mathcal{S}_E(x) : \mathbb{R}^{N_p} \to L^2(\mathbb{R}^3)$

$$\mathcal{S}_E(x)[u](r) := \sum_{j=1}^{N_p} S_a(x_j - r) u_j \tag{4}$$

and the interpolation operator $\mathcal{J}_E(x) : L^2(\mathbb{R}^3) \to \mathbb{R}^{N_p}$

$$(\mathcal{J}_E(x)[v])_i := \int_{\mathbb{R}^3} S_a(x_i - r) v(r) dr, \tag{5}$$

both of which are parameterized by $x \in \mathbb{R}^{N_p} \times \mathbb{R}^3$. These operators are adjoints of each other, so that for fixed $x \in \mathbb{R}^{N_p} \times \mathbb{R}^3$, any $u \in \mathbb{R}^{N_p}$, and any square integrable function v

$$\langle \mathcal{J}_E(x)[v], u \rangle_{\mathbb{R}^{N_p}} = \sum_{j=1}^{N_p} \left[\int_{\mathbb{R}^3} S_a(x_j - r) v(r) dr \right] u_j = \int_{\mathbb{R}^3} \left[\sum_{j=1}^{N_p} S(x_j - r) u_j \right] v(r) dr \tag{6}$$

$$= \int_{\mathbb{R}^3} \mathcal{S}_E(x)[u](r) v(r) dr = \langle v, \mathcal{S}_E(x)[u] \rangle_{L^2(\mathbb{R}^3)}. \tag{7}$$

The particle-in-cell (PIC) approach to compute the Coulomb force on particle i due to all the others consists of smoothing the collection of point charges with $\mathcal{S}_E$, solving Poisson's equation for the potential, taking the negative gradient of the potential, and then interpolating the result with $\mathcal{J}_E$. Let ϕ solve the Poisson equation

$$-\epsilon_0 \Delta \phi = (\mathcal{S}_E(x)[q]), \tag{8}$$

and define $E_P^i := -(\mathcal{J}_E(x)\,[\nabla\phi])_i$, where $\mathcal{J}_E$ acts on each component of $\nabla\phi$. The electrostatic force on particle i is then simply computed as

$$F_P^i = q_i E_P^i, \tag{9}$$

where the subscript P signifies that the quantities were computed from the solution to Poisson's equation. The numerical solution to (8) can be computed relatively quickly using standard Krylov subspace or spectral methods.

By linearity, the electric potential at a point y resulting from the solution to (8) is

$$\phi(y) = \frac{1}{\epsilon_0}(-\Delta)^{-1}\left(\sum_{j=1}^{N_p} q_j S_a(x_j - r)\right) \tag{10}$$

$$= \frac{1}{4\pi\epsilon_0}\sum_{j=1}^{N_p} q_j\, g(x_j, y), \tag{11}$$

where

$$g_a(x_j, y) := \int_{\mathbb{R}^3}\frac{S_a(x_j - r)}{|y - r|}dr. \tag{12}$$

For fixed y, the $1/|y-r|$ term in the integrand can be written as a multipole expansion about x_j, so that

$$\frac{1}{|y-r|} = \frac{1}{|y-x_j|} + \frac{(y-x_j)}{|y-x_j|^3}\cdot(r - x_j) + \psi(r, y - x_j), \tag{13}$$

where ψ represents the quadrupole, octopole, and higher order terms and decays as $|y - x_j|^{-5}$ or faster. Inserting the expansion into g_a gives

$$g_a(x_j, y) = \frac{1}{|y-x_j|} + \frac{y-x_j}{|y-x_j|^3}\cdot\int_{\mathbb{R}^3}(r-x_j)S_a(x_j - r)dr + \int_{\mathbb{R}^3}S_a(x_j - r)\psi(r, y - x_j)dr, \tag{14}$$

where the fact that S_a integrates to 1 is used. Further assume both here and below that S_a is symmetric, so that $S_a(-r) = S_a(r)\ \ \forall r \in \mathbb{R}^3$; it then has vanishing first moment

$$\int_{\mathbb{R}^3} r S_a(r)dr = 0, \tag{15}$$

and hence the dipole moment of ϕ will vanish. Therefore,

$$\phi(y) = \frac{1}{4\pi\epsilon_0}\sum_{j=1}^{N_p} q_j\left(\frac{1}{|y-x_j|} + \int_{\mathbb{R}^3}S_a(x_j - r)\psi(r, y - x_j)dr\right). \tag{16}$$

If the higher order terms in the multipole expansion are neglected, then ϕ is approximated by the sum of monopoles. If ϕ_M denotes this truncated potential, then the resulting electric field is

$$-\nabla\phi_M(y) = \frac{1}{4\pi\epsilon_0}\sum_{j=1}^{N_p}\frac{q_j}{|y-x_j|^3}(y - x_j). \tag{17}$$

Applying the interpolation operator $\mathcal{J}_E(x)$ to each vector component of (17) gives

$$-(\mathcal{J}_E(x)\,[\nabla\phi_M])_i = -\int_{\mathbb{R}^3}S_a(x_i - y)\nabla\phi_M(y)dy \tag{18}$$

$$= \frac{1}{4\pi\epsilon_0}\sum_{j=1,j\neq i}^{N_p}\int_{\mathbb{R}^3}S_a(x_i - y)\frac{q_j}{|y-x_j|^3}(y - x_j)dy; \tag{19}$$

note the $j = i$ term vanishes due to the assumed symmetry of S_a. Similar to above, the vector $(y-x_j)/|y-x_j|^3$ can be expanded about the point x_i:

$$\frac{y - x_j}{|y - x_j|^3} = \frac{x_i - x_j}{|x_i - x_j|^3} + \left[\nabla_y \left(\frac{y - x_j}{|y - x_j|^3} \right) \Bigg|_{y=x_i} \right] (y - x_i) + \Psi(y, x_i - x_j), \tag{20}$$

where, as before, Ψ represents higher order terms in the vector expansion. Since the second order tensor in brackets has no y-dependence, it can be brought outside the integral. Using again (15) and that S_a integrates to 1, (19) reduces to

$$- \left(\mathcal{J}_E(x) \left[\nabla \phi_M \right] \right)_i = \frac{1}{4\pi\epsilon_0} \sum_{j=1, j \neq i}^{N_p} \left(\frac{x_i - x_j}{|x_i - x_j|^3} + \int_{\mathbb{R}^3} S_a(x_i - y) \Psi(y, x_i - x_j) \, dy \right). \tag{21}$$

Ergo, if one again neglects the higher order terms built into Ψ, equality of (1) and (9) results, so that the electrostatic force on particle i computed by PIC approach is equal to the direct $\mathcal{O}(N_p^2)$ Coulomb calculation: $F_C^i = F_P^i$.

Of course, the equality of the two approaches is only approximate, and only correct to the extent that the ψ and Ψ terms in the Taylor expansions (13) and (20) are asymptotically small, which is true when pairs of point charges are well separated relative to the diameter a of the support of S_a:

$$\frac{|x_i - x_j|}{a} \gg 1. \tag{22}$$

In the case when (22) does not hold, it is easy to see that in general $F_C^i \neq F_P^i$. Consider a two particle system with charges q_1 and q_2 at the respective positions x_1 and x_2. For such a configuration, the Poisson equation (8) resulting from the PIC approach has solution

$$\phi(y) = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \frac{1}{|y - r|} \left(q_1 S_a(x_1 - r) + q_2 S_a(x_2 - r) \right) dr \tag{23}$$

with associated electric field

$$- \nabla \phi(y) = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} \frac{(y - r)}{|y - r|^3} \left(q_1 S_a(x_1 - r) + q_2 S_a(x_2 - r) \right) dr. \tag{24}$$

After applying the interpolation operator $\mathcal{J}_E(x)$, one obtains

$$F_P^1 = -q_1 \left(\mathcal{J}_E(x) \left[\nabla \phi \right] \right)_1 = \frac{1}{4\pi\epsilon_0} \int_{\mathbb{R}^3} q_1 S_a(x_1 - y) \int_{\mathbb{R}^3} \frac{(y - r)}{|y - r|^3} \left(q_2 S_a(x_2 - r) \right) dr \, dy \tag{25}$$

for the force on particle 1 due to particle 2 (note the particle exerts no force upon itself, again, by symmetry of S_a). A similar result holds for the total force on particle 2, F_P^2. In general, (25) is not equivalent to the standard Coulomb force (3); formally this only occurs in the limit $a \to 0$. Finally, note that if one makes the variable transforms $w = x_1 - r$ and $z = x_1 - y$, (25) becomes

$$F_P^1 = \frac{q_1 q_2}{4\pi\epsilon_0} \int_{\mathbb{R}^3} S_a(z) \int_{\mathbb{R}^3} \frac{(w - z)}{|w - z|^3} S_a(w - x_{12}) dw \, dz, \tag{26}$$

$x_{12} = x_1 - x_2$, which is the expression found in the classical text [1] by Hockney and Eastwood, as well as various papers in the physics/chemistry literature; see, for example, [2].

3   P3M

The above observations motivate a *mixed* approach for the efficient computation of the Coulomb forces on a collection of N_p point particles. It consists of solving the Poisson equation (8) from the PIC approach in order

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to efficiently calculate "far-field" forces, as well as performing a "short range", direct Coulomb calculation for all particles in a neighborhood of one another. An extra force calculation is needed, however, to correct for the fact that the PIC approach incorrectly captures the short range forces. The resulting procedure is termed the "particle-particle, particle-mesh" (P3M) method, described and analyzed in the classical text [1] of Hockney and Eastwood–see references therein for the historical development of the method.

Let

$$\Omega(i) := \{j \in \{1, \ldots, N_p\}, j \neq i | \operatorname{supp} S_a(x_i - \cdot) \cap \operatorname{supp} S_a(x_j - \cdot) \neq \emptyset\} \tag{27}$$

$$= \{j \in \{1, \ldots, N_p\}, j \neq i | \ |x_i - x_j| < 2a\} \tag{28}$$

define a local neighborhood of particle i. The total force on particle i in the P3M method is computed as

$$F_{P3M}^i = F_{SR}^i + F_{LR}^i - R^i, \tag{29}$$

that is, with a short-range, a long-range, and a correction "reference" force. The long range force is computed exactly as in PIC approach described above, so that for ϕ solving (8),

$$F_{LR}^i = -q_i \left(\mathcal{J}_E(x) \left[\nabla \phi \right] \right)_i \tag{30}$$

$$= \sum_{j=1, j \neq i}^{N_p} \frac{q_i q_j}{4\pi\epsilon_0} \int_{\mathbb{R}^3} S_a(x_i - y) \int_{\mathbb{R}^3} \frac{(y - r)}{|y - r|^3} S_a(x_j - r) dr \, dy. \tag{31}$$

The short range force is given as

$$F_{SR}^i = \sum_{j \in \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \frac{(x_i - x_j)}{|x_i - x_j|^3}, \tag{32}$$

and the correction force is simply

$$R^i = \sum_{j \in \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \int_{\mathbb{R}^3} S_a(x_i - y) \int_{\mathbb{R}^3} \frac{(y - r)}{|y - r|^3} S_a(x_j - r) dr \, dy \tag{33}$$

$$= \sum_{j \in \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \int_{\mathbb{R}^3} S_a(z) \int_{\mathbb{R}^3} \frac{(w - z)}{|w - z|^3} S_a(w - x_{ij}) dr \, dy \tag{34}$$

For efficiency, the correction force R^i is pre-computed and tabulated for fixed S_a as a function of $x_{ij} = x_i - x_j$. For appropriately chosen smoothing function S_a, R^i can be treated (approximately) as a function of the separation distance $|x_{ij}|$ only, hence reducing the dimensionality of the "reference" table.

Inserting each force (30), (32), (33) into the expression (29) gives

$$F_{P3M}^i = \sum_{j \in \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \frac{(x_i - x_j)}{|x_i - x_j|^3} \tag{35}$$

$$+ \sum_{j \notin \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \int_{\mathbb{R}^3} S_a(x_i - y) \int_{\mathbb{R}^3} \frac{(y - r)}{|y - r|^3} S_a(x_j - r) dr \, dy. \tag{36}$$

Making use of multipole expansions in the same manner as (13) and (20) above,

$$F_{P3M}^i = \sum_{j \in \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \frac{(x_i - x_j)}{|x_i - x_j|^3} + \sum_{j \notin \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \frac{(x_i - x_j)}{|x_i - x_j|^3} \tag{37}$$

$$+ \sum_{j \notin \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \int_{\mathbb{R}^3} S_a(x_i - y) \left(\Psi(y, x_i - x_j) + \int_{\mathbb{R}^3} S_a(x_j - r) \nabla_y \psi(r, y - x_j) dr \right) dy \tag{38}$$

$$= F_C^i + \sum_{j \notin \Omega(i)} \frac{q_i q_j}{4\pi\epsilon_0} \int_{\mathbb{R}^3} S_a(x_i - y) \left(\Psi(y, x_i - x_j) + \int_{\mathbb{R}^3} S_a(x_j - r) \nabla_y \psi(r, y - x_j) dr \right) dy. \tag{39}$$

Hence, in theory, the force on each particle i resulting from the P3M method is equivalent to Coulomb force (1), up to the size of the terms higher order terms Ψ (respectively ψ) in the multipole vector (resp. scalar) expansions of the singular integral kernels.

References

[1] R. W. Hockney and J. W. Eastwood. *Computer Simulation Using Particles.* Taylor & Francis, Inc., Bristol, PA, USA, 1988.

[2] S. Aboud, D. Marreiro, M. Saraniti, and R. Eisenberg. A poisson p3m force field scheme for particle-based simulations of ionic liquids. *Journal of Computational Electronics*, 3(2):117–133, Apr 2004.