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An Optimization Model of Molecular Voronoi Cells in Computational Chemistry

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ABSTRACT

In computational chemistry or crystallography, we always meet the problem that requires distributing N particles in one square cell with the minimal neighbour distance. Sometimes this problem is with special or complex constraints. This short article will build a molecular optimization model for the problem, and then will show one example of the application of this model.

INTRODUCTION

We consider the problem that requires distributing N (≥ 1) particles in one three- dimensional (3D) $2a \times 2b \times 2c$ box/cell/unit with the minimal neighborhood distance. Let us define that d_{ij} is the direct-distance variable between particle i ($1 \leq i \leq N$) and particle j ($1 \leq i \leq N, j \neq i$).

Direct-distance means particles i and j have a direct interaction relationship, for example, in computational chemistry, VanderWaals (vdW) contact [1,2], (or) solvent accessible surface area (ASA) contact (en.wikipedia.org/wiki/Accessible surface area), etc to each other. Denote (x_{i1}, x_{i2}, x_{i3}) and (x_{j1}, x_{j2}, x_{j3}) the coordinates of particles i and j, respectively. Then, for the convenience of practical computations [3,4], we can build an optimization model for the above problem.

$$min\ f(x) = \left(\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} d_{ij} \right)^2 \tag{1}$$

$$= \left(\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} (x_{i1} - x_{j1})^2 + (x_{i2} - x_{j2})^2 + (x_{i3} - x_{j3})^2 \right)^2 \tag{2}$$

$$Subject\ to \quad -a \leq x_{i1}, x_{j1} \leq a, -b \leq x_{i2}, x_{j2} \leq b, -c \leq x_{i3}, x_{j3} \leq c,\ i, j = 1, \ldots, N. \tag{3}$$

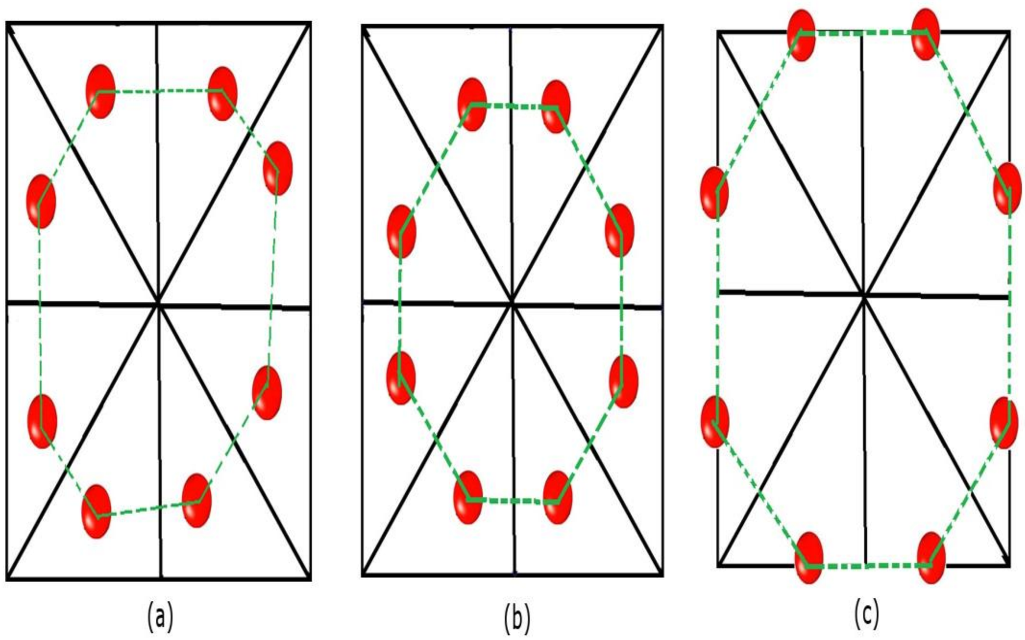
This might be a problem of Voronoi diagram (en.wikipedia.org/wiki/Voronoi diagram) and the unit is called Voronoi cell. In computational chemistry, some crystals own special structures of the Voronoi cells; in such a case, we may add some additional constraints to **Equation (3).**

Clearly, the well-known Lennard-Jones Clusters problem [2] is one case of the above optimization problem **Equations (1–3).**

Example

We give a 2D Voronoi cells example **Figure 1.** We distribute 8 particles in one 2D square with the minimal neighborhood distance among them, with a constraint that each particle is only in one of the 8 Voronoi cells of the square. **Figure 1(a)** shows the initial solution that is given to the problem. **Figure 1(b)** and **Figure 1(c)** show the optimal (octagon) distribution of the 8 particles inner the square and onto the boundary of the square, respectively, after we solve the optimization problem Equations. (1-3) if in Equation. (3) "≤" is "≤" **Figure 1(b)** or "<" **Figure 1(c).**

Figure 1: The optimization model to distribute 8 particles into 8 Voronoi cells of a square unit: (a) initial distribution given, (b) optimal (octagon) distribution inner the square, and (c) Optimal (octagon) distribution onto the boundary of the square. The green dashed line denotes there is a direct relationship between the two particles they link (e.g. the two atoms have the vdW interactions).



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REFERENCES

1. Olechnovic K, et al. A fast and reliable tool for computing the vertices of the Voronoi diagram of atomic balls. J Comput Chem.2014;35:672-681.
2. Zhang JP. The hybrid idea of optimization methods applied to the energy minimization of (prion) protein structures focusing on the β2–α2 loop. Biochem Pharmacol (Los Angel) 2015;1:10.
3. Zhang JP, et al. A novel canonical dual computational approach for prion AGAAAAGA amyloid fibril molecular modeling. J Theor Biol.2011;284:149–157.
4. Zhang JP. The LBFGS quasiNewtonian method for molecular modeling prion AGAAAAGA amyloid fib- rils. Nat Sci 4(12A) (Special Issue on Bioinformatics, Proteomics, Systems Biology and Their Impacts to Biomedicine). 2011;1:1097–1098.