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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 unit with the minimal neighbor 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.

Keywords: Computational chemistry; Crystal molecular structure; Optimization model; Optimized Voronoi cells distribution

We consider the problem that requires distributing N (≥ 1) particles in one three - dimensional (3D) 2a × 2b × 2c box/cell/unit with the minimal neighborhood distance. Let us define that d_{ij} is the direct-distance variable between particle i ($1 \le i \le N$) and particle j ($1 \le i \le N$, $j \ne i$). Direct-distance means particles i and j have a direct interaction relationship, for example, in computational chemistry, the van der Waals (vdW) contact [1], or solvent accessible surface area (ASA) contact, 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 [2,3], we can build an optimization model for the above problem:

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

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

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

This might be a problem of 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 Eq. (3). Clearly, the well-known Lennard-Jones Clusters problem [4] is one case of the above optimization problem Eqs. (1) ~ (3). Some computer-aided design models can be looked as the problem Eqs. (1) ~ (3) [5,6,7]. Any optimization algorithms can be used to solve Eqs. (1) ~ (3) but global optimization algorithms (e.g., in [8]) are more preferred to use.

Example 1: We give a 2D Voronoi cells example (Figure 1). 2D is a special case of 3D. 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 Eqs. (1) ~ (3).

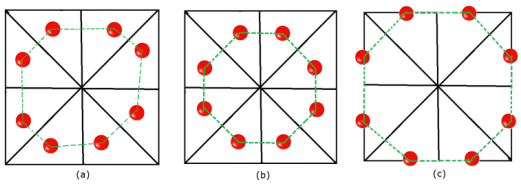

Figure 1: The optimization model to distribute 8 particles into 8 Voronoi cells of a square unit: (a) initial distribution given, (b) optimal (octagon) distribution inner the square, and (c) optimal (octagon) distribution onto the boundary of the square. The green dashed line denotes there is a direct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

Example 2: We give a 3D Voronoi cells example (movies in [9]). The Lennard-Jones clusters problem is clearly a 3D Voronoi cells problem. Cameron et al. presented 4 movies to illuminate how the atoms to be arranged and at last reach the minimal energy states [9].

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