An Optimization Model of Molecular Voronoi Cells in Computational Chemistry

Jia pu Zhang1,2*
1Molecular Model Discovery Laboratory, Department of Chemistry and Biotechnology, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Hawthorn Campus, Hawthorn, Victoria 3122, Australia
2Graduate School of Sciences, Information Technology and Engineering and Centre of Informatics and Applied Optimization, Faculty of Science, The Federation University Australia, Mount Helen Campus, Mount Helen, Ballarat, Victoria 3353, Australia

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 ≤ i ≤ N) and particle j (1 ≤ j ≤ N, j ≠ 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:

\[
\begin{align*}
\min f(x) &= \left( \sum_{i=1}^{N} \sum_{j=1}^{N} d_{ij}^2 \right)^{1/2} \quad (1) \\
&\quad - \left( \sum_{i=1}^{N} \sum_{j=1}^{N} (x_{i1}-x_{j1})^2 + (x_{i2}-x_{j2})^2 + (x_{i3}-x_{j3})^2 \right)^{1/2} \quad (2) \\
&\quad - a \leq x_{i1}, x_{j1} \leq a, -b \leq x_{i2}, x_{j2} \leq b, -c \leq x_{i3}, x_{j3} \leq c, i, j = 1, ..., N \quad (3)
\end{align*}
\]

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).

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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*Corresponding author: Jia pu Zhang, Molecular Model Discovery Laboratory, Department of Chemistry and Biotechnology, Faculty of Science, Engineering and Technology, Swinburne University of Technology, Hawthorn Campus, Hawthorn, Victoria 3122, Australia, Tel: +61-3-9214-5596; +61-3-5327-6335; E-mail: jiapuzhang@swin.edu.au; j.zhang@federation.edu.au

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