Reliable global optimization on atom clusters

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Given a cluster of n atoms define $x_i \in \mathbb{R}^3$ $(i = 1, \ldots, n)$ as the center of the ith atom. The potential energy function of the cluster $x = (x_1, \ldots, x_n) \in \mathbb{R}^{3n}$ is defined by the summation of the two-body inter-particle pair potentials over all of the pairs, i.e.

$$E(x) = \sum_{i<j} v(\|x_i - x_j\|) \quad (i, j = 1, \ldots, n)$$

where $\|.\|$ is the Euclidean distance and $v : \mathbb{R} \to \mathbb{R}$ is the pair-potential function. The global optimization of a potential energy function describing an atom cluster is a challenge for the scientific computing. Recently many papers deal with this problem, especially the so called Lennard-Jones problem, where the pair-potential function is defined as

$$v(r) = \frac{1}{r^{12}} - \frac{2}{r^6}$$

where r is the atom-pair distance. However, one can find no paper about reliable method for finding the optimal structure of Lennard-Jones atom clusters. Branch-and-bound type methods based on interval arithmetic could produce reliable solution for global optimization problems. In this talk the Lennard-Jones atom cluster problem will be considered with the reliable point of view. First, we establish good lower bound for the minimal inter-atomic distance in the optimal structure (independently from the number of atoms). From this result a guaranteed lower bound for the global optimum will be given which is a linear function of the number of atoms. Using this results and geometrical considerations we will introduce an optimization method producing guaranteed globally optimal solutions.