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An iterative procedure for finding locally and globally optimal arrangements of particles on the unit sphere☆

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ABSTRACT

The problem of determination of globally optimal arrangements of N pairwise-interacting particles arises in a variety of biological, physical, and chemical applications. At the same time, the important related question of finding all, or many, local minima of the corresponding energy functions, and the study of structure of these minima, has received relatively little attention.

A computational procedure is proposed to compute locally optimal and putative globally optimal arrangements of N particles constrained to a sphere. The procedure is able to handle a wide class of pairwise potentials, and can be generalized to other kinds of surfaces and interactions.

As computational examples, locally and globally energy-minimizing arrangements of particles on the unit sphere, interacting via the Coulombic, logarithmic, and inverse square law potentials, are computed. We present new results for the logarithmic potential consisting of 45 new local minima for $N \leq 65$ and two new global minima ($N = 19, 46$), as well as results for the inverse square law potential which has not previously been studied. We provide comprehensive tables of all minima found, and exclude saddle points. The algorithm can perform computations exceeding $N = 100$ with reasonable execution times.

Program summary

Program Title: EOPS 1.0 - Energy Optimizer for Particles on the Sphere
Program Files doi: `http://dx.doi.org/10.17632/cbn8jt2ffw.1`
Licensing provisions: GPLv3
Programming language: MATLAB 2015b, C++98, Maple
Nature of problem: Computation of locally and globally optimal arrangements of N particles on the sphere for different pairwise potentials. This constitutes a constrained local optimization problem with $2N - 3$ degrees of freedom.
Solution method: For N particles, the pairwise potential energy is minimized via steepest descent trajectory from a starting configuration generated from known putative $(N - 1)$-particle optimal configurations.
Restrictions: Spherical domain in $\mathbb{R}^3$ and pairwise potentials. The number of particles is limited by the computing power and memory of the machine.
Unusual features: The programs are executed from MATLAB scripts which call C++ and Maple procedures which perform the bulk of the computations.

1. Introduction

The general problem of finding optimal arrangements of particles on the boundary of a domain in $\mathbb{R}^n$ dates back over 100 years to the Thomson problem, which concerns finding the arrangement of N identically charged particles on the surface of a sphere in $\mathbb{R}^3$ that minimizes the Coulombic energy. This problem arose in J.J. Thomson's early "plum pudding" model of the atom in which the electrons are point charges that are suspended in a "jellium" of positive charge. Similar problems now arise in molecular biophysics and material science.

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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An *optimal configuration* is defined as follows. Given a domain $\mathcal{D}$ in $\mathbb{R}^n$, $n \geq 2$, an arrangement of N identical particles is said to be an optimal configuration when the set of particle coordinates $\{\mathbf{x}_i\}_{i=1}^N$ minimizes the pairwise potential,

$$\mathcal{H}(\mathbf{x}_1, ..., \mathbf{x}_N) = \sum_{i<j}^{N} h(|\mathbf{x}_i - \mathbf{x}_j|), \tag{1.1}$$

under the constraint $\mathbf{x}_i \in \partial\mathcal{D}$ where h is a pairwise energy associated with a single pair of particles. One obtains the Thomson problem when h is the Coulombic potential

$$h(d) = \frac{1}{d}. \tag{1.2}$$

Finding optimal configurations constitutes a constrained local optimization problem in which the objective function is given by (1.1).

The problem of distributing points on the boundary of a domain has applications in the *narrow escape problem* in biophysics. In this problem, a Brownian particle diffuses inside of a bounded domain with a reflecting boundary except for N small absorbing "traps", or windows. The problem consists in finding the mean first passage time (MFPT) of Brownian particles through the traps. Narrow escape problems can be used to model the motion of Brownian particles (proteins, ions, etc.) which must exit a confining domain in order to accomplish a biological function. Some examples include chemical reactions in microdomains (such as synapses and microvesicles) [1], the time required for diffusive particles inside a biological cell to react with proteins on the cell membrane [2], the dynamics of receptors undergoing Brownian motion on the cell membrane [3], and virus transport inside the cell nucleus [4]. A specific example of a narrow escape problem for the sphere is a model of a biological microstructure known as a dendritic spine (see [1] and references therein). These structures are found in neurons as the postsynaptic part of a synapse and consist of a head at the end of a long neck. The mean time for a calcium ion undergoing Brownian motion to escape the spine head (i.e. the MFPT) is an important quantity related to synaptic plasticity.

Multi-term asymptotic expressions for the MFPT have recently been obtained for various domains using the method of matched asymptotic expansions [5–7]. In the case where the domain is a sphere in $\mathbb{R}^3$ with N small absorbing spherical caps on the boundary, it has been shown [5,8] that finding arrangements of traps that minimize the average MFPT requires minimization of an energy-like function given by (1.1) over the surface of the sphere where

$$h(d) = \frac{1}{d} - \frac{1}{2}\log d - \frac{1}{2}\log(2+d). \tag{1.3}$$

A related problem, known as the *narrow capture problem*, involves finding the MFPT for a Brownian particle diffusing inside a domain with a reflecting boundary but small absorbing interior targets. This problem also has applications in molecular biophysics (see [9] and references therein). The case of a general domain with a single interior target consisting of absorbing spherical caps on an otherwise reflecting boundary has been studied recently [10,11]. In particular, it was shown that when the target is spherical with N absorbing circular pores, the MFPT is minimized when the target is at the center and the arrangement of pores minimizes a pairwise energy-like function in which the pairwise energy is similar to (1.3)

$$h(d) = \frac{1}{d} + \frac{1}{2}\log\left(\frac{d}{2+d}\right). \tag{1.4}$$

Computation of optimal configurations also relates to packing problems. The best-packing problem for the sphere consists of finding the most efficient way of packing circles (spherical caps) onto the surface of a sphere, or equivalently maximizing the smallest radius of N circles on the sphere. This problem is also referred to as the Tammes problem after the Dutch botanist who studied the arrangement of exit places on grains of pollen [12]. Recently this problem has been solved exactly for $N = 13, 14$ [13], and exact solutions are now known for all N up to 14. The arrangements of spherical caps minimize an extremely short-range energy function (see [14] and references therein) which is given by the limiting case

$$h(d) = \frac{1}{d^m}, \qquad m \to \infty. \tag{1.5}$$

In the low-temperature limit, the geometry of a crystalline material is determined by the lowest energy configuration or "ground-state" of the system. The ground state configurations for planar crystals contain no defects in their structure, however, in general this is impossible for non-planar crystals due to the Euler theorem of topology. The geometry and arrangements of defects in such materials play a role in determining their electrical and mechanical properties. As a well-known example of a crystal with non-planar geometry, consider carbon nanotubes (CNTs). The chirality of a CNT determines whether it is eclectically conducting, insulating, or semiconducting.

Spherical structures occur frequently in material science, notably the class of carbon fullerene molecules discovered in 1985 [15]. Spherical structures also occur in colloidosomes which are shells consisting of colloidal particles surrounding a liquid center. The arrangements of charged colloids correspond to solutions of the Thomson problem[16]. The Thomson problem also serves as a reasonable model of multielectron bubbles in liquid helium [16,17]. These bubbles are formed above the liquid surface when an electrode is submerged in the liquid and the electric field strength is increased beyond a critical value. This causes electrons that are initially outside the surface to enter the liquid via formation of multielectron bubbles. The bubbles contain approximately 10^5 to 10^8 electrons spread across the surface and the bubble radius is between 10 μm and 100 μm. The inter-electron spacing is usually at least 0.2 μm and therefore the electrons can be considered classical particles distributed such that the Coulomb energy is minimized [17–19]. Furthermore, it has been shown that a spherical bubble is energetically stable against perturbations under an appropriately pressure [20]. Thus multielectron bubbles indeed closely resemble Thomson's original problem albeit in a different context.

The Thomson problem today remains interesting both as a mathematical problem but also as a benchmark for testing optimization software. A comprehensive list of putative globally energy-minimizing designs has been produced for all N up to 132 and some selected N up to 282 [21]. Local minima are not as well known, although many putative local minima have been discovered up to $N = 112$ [22] and up to $N = 150$ for a few selected N [23]. Putative global minima for particles interacting via the logarithmic potential have also been studied

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