Local and Global Optimization of Particle Locations on the Sphere: Models, Applications, Mathematical Aspects, and Computations

Alexei F. Cheviakov, Wesley Ridgway
University of Saskatchewan, Saskatoon, Canada

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Outline

1. Problem and Motivation
2. Geometry and Typical Results
3. Some Questions of Interest
4. Local and Global Optimization: a Numerical Method
5. Computational Results
6. Highlights and Open Problems
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The Global Optimization Problem

Problem:

- Global optimization of some objective function that depends on positions of small "particles", or "pores", or "traps", on the surface of a 3D domain:

\[
\min \mathcal{H}(x_1, \ldots, x_N), \quad x_i \in \partial V, \quad V \subset \mathbb{R}^3.
\]
Motivation: Example 1, Thomson problem

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- Total Coulombic interaction energy:

\[
\mathcal{H}_C(x_1, \ldots, x_N) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} h(x_i, x_j)
\]

- Pairwise energy function:

\[
h(x_i, x_j) = \frac{1}{|x_i - x_j|}
\]
Motivation: Example 2, Narrow Escape Problems

- Example 2: Chemical exchange through nuclear pores
Motivation: Example 2, Narrow Escape Problems

- **Example 2: Chemical exchange through nuclear pores**
  - Typical nucleus size: $\sim 6 \times 10^{-6}$ m; pore size $\sim 10^{-8}$ m.
  - $\sim 2000$ nuclear pore complexes in a typical nucleus
  - mRNA, proteins, smaller molecules
  - $\sim 1000$ translocations per complex per second
  - Trap separation $\sim 5 \times 10^{-7}$ m

**A Narrow Escape Problem:**
- Diffusion / Brownian motion;
- High passage rates;
- Well-separated small surface traps.

- Similar mechanisms for ion pumps, like Na$^+$-K$^+$ pumps, etc.
The MFPT Problem

The setup:

- A Brownian particle confined in a domain $\Omega \in \mathbb{R}^3$.
- Initial position: $x \in \Omega$.
- Mean First Passage Time (MFPT): $v(x)$.
- Domain boundary: $\partial \Omega = \partial \Omega_r$ (reflecting) $\cup$ $\partial \Omega_a$ (absorbing).
- $\partial \Omega_a = \bigcup_{i=1}^{N} \partial \Omega_{\varepsilon_i}$: small absorbing traps (size $\sim \varepsilon$).
The MFPT Problem

Problem for the MFPT $v = v(x)$ \cite{Holcman, Schuss (2004)}:

$$\begin{cases}
\triangle v = -\frac{1}{D}, & x \in \Omega, \\
v = 0, & x \in \partial \Omega_a; \quad \partial_n v = 0, & x \in \partial \Omega_r.
\end{cases}$$

Average MFPT: $\bar{v} = \frac{1}{|\Omega|} \int_{\Omega} v(x) \, dx = \text{const.}$
Escape Problems and Brownian Dynamics: Some References


An Asymptotic Solution of the MFPT Problem for the Sphere

Asymptotic assumptions:
- \( D = \text{const}; \)
- Domain: a unit sphere;
- \( N \) equal traps of radius \( \varepsilon \ll 1. \)

An asymptotic result for the average MFPT [A.C., M.Ward, R.Straube (2010)]:

\[
\bar{v} \sim \frac{|\Omega|}{4\varepsilon DN} \left[ 1 + \frac{\varepsilon}{\pi} \log \left( \frac{2}{\varepsilon} \right) + \frac{\varepsilon}{\pi} \left( -\frac{9N}{5} + 2(N - 2) \log 2 + \frac{3}{2} + \frac{4}{N} \mathcal{H}_{MFPT} \right) \right];
\]

\[
\mathcal{H}_{MFPT}(x_1, \ldots, x_N) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} h(x_i, x_j),
\]

\[
h(x_i, x_j) = \frac{1}{|x_i - x_j|} - \frac{1}{2} \log |x_i - x_j| - \frac{1}{2} \log (2 + |x_i - x_j|)
\]

Similar results exist for non-spherical domains, non-equal traps;

An asymptotic formula for the actual MFPT \( v = v(x) \) is also known.
Motivation: Example 3, Power and Logarithmic Interactions

- General power pairwise interaction potentials, same particles:

\[ \mathcal{H}_n(x_1, \ldots, x_N) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} h(x_i, x_j), \quad h(x_i, x_j) = |x_i - x_j|^{-n}. \]

- Logarithmic potential:

\[ \mathcal{H}_{\text{log}}(x_1, \ldots, x_N) = -\sum_{i=1}^{N} \sum_{j=i+1}^{N} \log |x_i - x_j|. \]

- Various applications, including the study of vortex defects in a liquid crystal confined to a closed surface with spherical topology [Bergersen et al (1994) and references therein].
Problem and Motivation

Geometry and Typical Results

Some Questions of Interest

Local and Global Optimization: a Numerical Method

Computational Results

Highlights and Open Problems
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\[
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\]

- The vast majority of results pertain to the 2-sphere \( \partial V = S^2 \) (“spherical designs”).

- Virtually all results describe optimal configurations of identical particles.

- In some works, scaling laws are derived for a fixed total trap area as \( N \to \infty \).
Results: a Very Brief Overview

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\[ \min \mathcal{H}(x_1, \ldots, x_N), \quad x_i \in \partial V, \quad V \subset \mathbb{R}^3. \]

The global optimization problem: features and progress
- A high-dimensional problem; \(2N\) degrees of freedom in \(\mathbb{R}^3\) (\(2N - 3\) for \(S^2\)).
- No exact solutions except for cases with high symmetry, in particular, sphere in \(n > 3\) dimensions [e.g., Cohn & Kumar (2006)];
- "Black box" software: standard approaches (genetic algorithms, simulated annealing, dynamical systems, etc.)
- Potential- and domain-specific software.
- In the literature, putative numerical global minima are presented; virtually no works discuss local minima [Erber & Hockney (1996)].
Geometrical Features and Questions

- A long-standing problem of "uniformly meshing" a sphere (or another domain).
- How does one distinguish two similar/close configurations?
  - Energy values themselves are insufficient.
  - Particularly important in symmetric domains.
- Universally optimal configurations holding for a wide class of potentials? [Spheres in $\mathbb{R}^n$: e.g., Cohn & Kumar (2006).]
Coordination number $c_i$ of a particle: number of neighbours (usually $c_i = 6$).

Topological constraints: Euler's Theorem, $V - E + F = 2$; can show that

$$\sum_i (6 - c_i) = 12,$$

where $(6 - c_i)$ is the “topological charge”.

Figure 16. Results of a minimization of 500 particles interacting with a Coulomb potential, showing the appearance of scars.
At least 12 particles with five-fold coordination.

A **scar**: a cluster of particles where \( c_i \neq 6 \).

For the same \( N \), different configurations may or may not have different scar pictures.

Applications: 2D matter; defects play an essential role in describing crystalline particle packings on the sphere.
three runs were started from different random starting configurations and continued until all three runs had located the same lowest minimum. This procedure required up to 200,000 basin-hopping steps in some cases. Previous experience with many different systems, including cross validation of basin-hopping results by other methods, suggests that the resulting structures are good candidates for the true global minima. However, we note that exceptions could arise for multifunnel potential energy surfaces, as documented in previous work. The results are recorded in Table I and selected structures are illustrated in Fig. 1. Nine of these structures improve upon previous results by between $10^{-4}$ and 18 a.u. No isolated disclinations are found in this data set for $N = 520$. It is also noteworthy that most global minima have nontrivial point groups, in agreement with the suggestion that higher-symmetry structures are generally associated with particularly high or particularly low energies. We expect this trend to extend to larger systems with defects separating into 12 distinct groups related by exact or approximate symmetry operations. This pattern may also help to minimize strain, in an analogous fashion to the pentagon "repulsion" rule for fullerenes.

Most of the defects for $N = 1152$ are again twinned grain boundaries, but we also see a defect with an alternating arrangement of pentagons, hexagons, and heptagons colored red, medium gray, green, light gray, and blue, respectively.

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A Numerical Method for Local and Global Optimization

- Implemented mainly in Matlab.
- Start from $N = 4$: tetrahedron.
A Numerical Method for Local and Global Optimization

where \( n \) is user specified and should be an array (see appendix B). Note that the choice is not required to be the same as the potential used in the optimization algorithm. Thus each configuration has a vector of pairwise energies, each element of which corresponds to a choice of \( n \). Denote the \( k \)th vector in a given cluster as \( E(k) \).

3. For each of the \( m \) clusters, sort each energy vector in ascending numerical order. Then normalize each element following the same procedure as in algorithm 1. The resulting arrays are denoted \( \tilde{E}(k) \).

4. For each of the \( m \) clusters found in 1), cluster the configurations within each based on energy. As in the first algorithm, the tolerance, \( \delta \) can either be set explicitly by the user or 'automatically' by the program. When set automatically, the tolerance is

\[
\delta = |\text{tol}| \times \max_k |\tilde{E}(k)| \quad (2.9)
\]

where \( \text{tol} \) is again a parameter specified by the user (see appendix B). All configurations within an energy cluster will be equivalent given a suitable tolerance.

As with algorithm 1, suitable tolerances are chosen through experimentation.

2.3 The Starting Configurations

The local optimization routine requires an initial configuration of particles. Previous work has focused on using many trials with random starting configurations. This quickly becomes computationally expensive as the number of local minima is believed to increase exponentially \([?]\) which requires the number of random trials to increase quickly as well. A unique algorithm for generating starting configurations was developed that significantly reduces the number of optimizations.

Starting configurations: Introduce, one by one, triangle middles. Remove redundant configurations.
For each starting configuration, perform local optimization (C++).

Remove redundant configurations.

Remove saddle points (Maple).

Repeat $N \rightarrow N + 1$. 
Geometrical symmetries!
Removing Redundant Configurations

- Geometrical symmetries!

- **Coordinate-invariant characteristics of a configuration**: energy; pairwise distances; pairwise energies...
Geometrical symmetries!

**Coordinate-invariant characteristics of a configuration**: energy; pairwise distances; pairwise energies...

Many details will be given in the next talk.
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Computational Results: Coulomb Potential, $N \leq 65$

- Number of locally optimal configurations found for the Coulomb potential.
Computational Results: Coulomb Potential, $N \leq 65$

All Normalized Minima Energies

- Relative Coulomb energy spectrum.
Computational Results: Logarithmic Potential, $N \leq 65$

- Number of locally optimal configurations found for the Logarithmic potential.
Relative Logarithmic energy spectrum.
Computational Results: Inverse Square Law Potential, $N \leq 65$

- Number of locally optimal configurations found for the Inverse Square Law potential.
Computational Results: Inverse Square Law Potential, $N \leq 65$

- Relative Inverse Square Law energy spectrum.
Computational Results: Inverse Square Law Potential, $N \leq 65$

Six local minima for the inverse square law, $N = 60$. 

A. Cheviakov, W. Ridgway (UofS, Canada) 
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## Main findings

- Local and global minima and respective configurations of identical particles for Coulomb, Logarithmic, and Inverse Square Law potentials.
- Coordination numbers and energy spectra computed.
- No special scar picture characterizes global minima.
- Saddles consistently arise in numerical dynamical system-based local optimization; can be systematically excluded.

## Ongoing & future work

- Computations for higher $N$.
- Similar computations for the MFPT potential.
- Local minima for non-equal interacting particles?
Spherical trap configurations for $2N = 8$ traps of two kinds with radius ratio 10. The global minimum of the average MFPT $\bar{\nu}$. (b), (c): nearby local minima [C., Reimer, Ward (2012)].
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