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

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May 25, 2017

Outline

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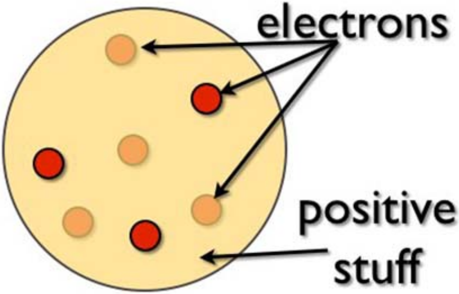
The Global Optimization Problem

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:

$$\min \mathcal{H}(\mathbf{x}_1, \ldots, \mathbf{x}_N), \qquad \mathbf{x}_i \in \partial V, \qquad V \subset \mathbb{R}^3.$$

- Example 1: Thomson problem



- Example 1: Thomson problem

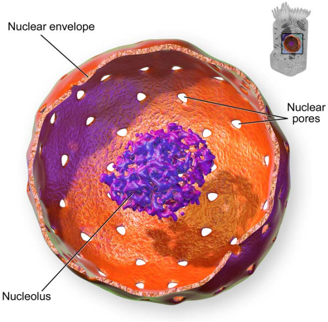
- Total Coulombic interaction energy:

$$\mathcal{H}_C(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} h(\mathbf{x}_i, \mathbf{x}_j)$$

- Pairwise energy function:

$$h(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{|x_i - x_j|}$$

- 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.
- ~ 2000 nuclear pore complexes in a typical nucleus
- mRNA, proteins, smaller molecules
- ~ 1000 translocations per complex per second

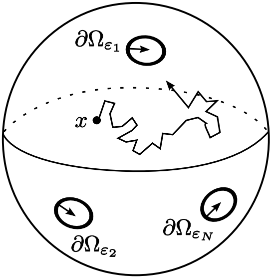
- Trap separation $\sim 5 \times 10^{-7}$ m

A Narrow Escape Problem:

- Diffusion / Brownian motion;
- High passage rates;
- Well-separated small surface traps.

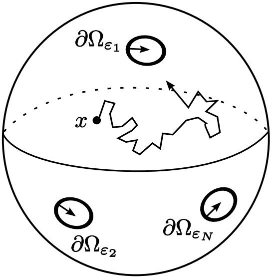
- Similar mechanisms for ion pumps, like Na^{+}-K^{+} pumps, etc.

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 $\sim \varepsilon$).



Problem for the MFPT $v = v(x)$ [*Holcman, Schuss (2004)*]:

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

Average MFPT: $\bar{v} = \dfrac{1}{|\Omega|} \displaystyle\int_\Omega v(x)\, dx = \text{const.}$

Escape Problems and Brownian Dynamics: Some References

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An Asymptotic Solution of the MFPT Problem for the Sphere

Asymptotic assumptions:

- $D = \mathrm{const}$;
- 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)*]:

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

$$\mathcal{H}_{MFPT}(\mathbf{x}_1, \dots, \mathbf{x}_N) = \sum_{i=1}^{N}\sum_{j=i+1}^{N} h(\mathbf{x}_i, \mathbf{x}_j),$$

$$h(\mathbf{x}_i, \mathbf{x}_j) = \frac{1}{|x_i - x_j|} - \frac{1}{2}\log|x_i - x_j| - \frac{1}{2}\log\left(2 + |x_i - x_j|\right)$$

- 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:

$$\mathcal{H}_n(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} h(\mathbf{x}_i, \mathbf{x}_j), \qquad h(\mathbf{x}_i, \mathbf{x}_j) = |x_i - x_j|^{-n}.$$

- Logarithmic potential:

$$\mathcal{H}_{log}(\mathbf{x}_1, \ldots, \mathbf{x}_N) = -\sum_{i=1}^{N} \sum_{j=i+1}^{N} \log |x_i - x_j|.$$

- 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*].

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Results: a Very Brief Overview

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:

$$\min \mathcal{H}(\mathbf{x}_1, \ldots, \mathbf{x}_N), \qquad \mathbf{x}_i \in \partial V, \qquad V \subset \mathbb{R}^3.$$

- 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 $N \to \infty$.

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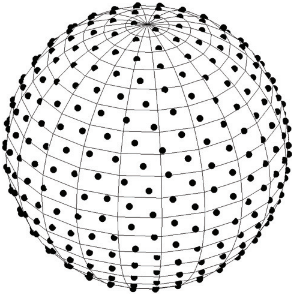
The global optimization problem: features and progress

- 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



436 traps

- 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)*.]

Geometrical Features and Questions

488 *M.J. Bowick and L. Giomi*

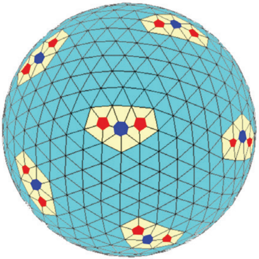


Figure 16. Results of a minimization of 500 particles interacting with a Coulomb potential, showing the appearance of scars.

- 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".

Geometrical Features and Questions

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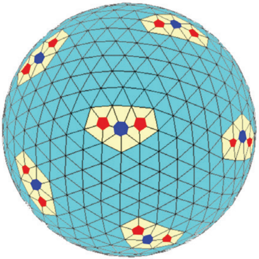
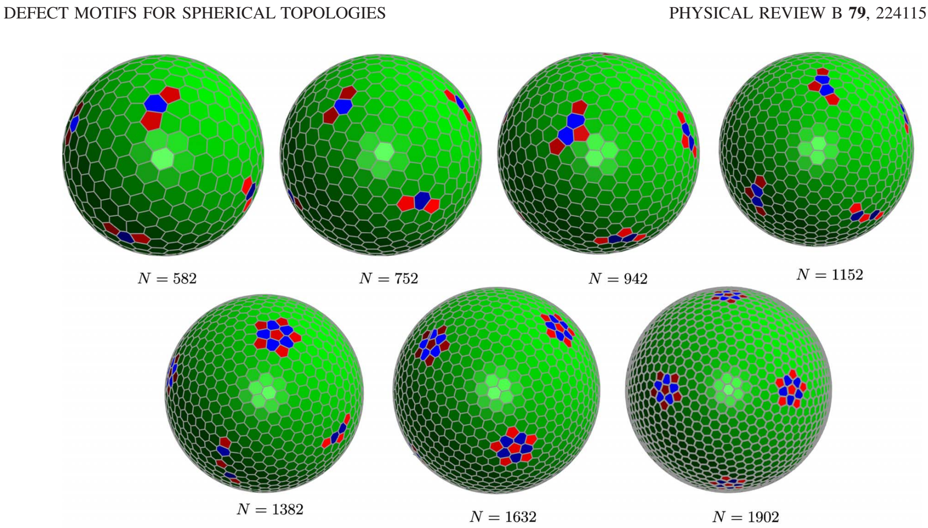


Figure 16. Results of a minimization of 500 particles interacting with a Coulomb potential, showing the appearance of scars.

- 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.

Geometrical Features and Questions



From *Wales et al (2009)*.

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- How many local minima can one expect for a given N and a given potential, typically?
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- What is the comparative scar geometry for various local and global minima?
- The "simplest" domain: unit sphere. Not much is known!

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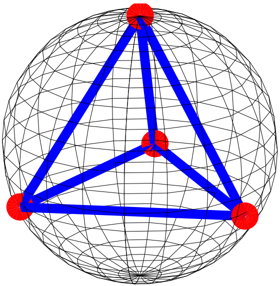
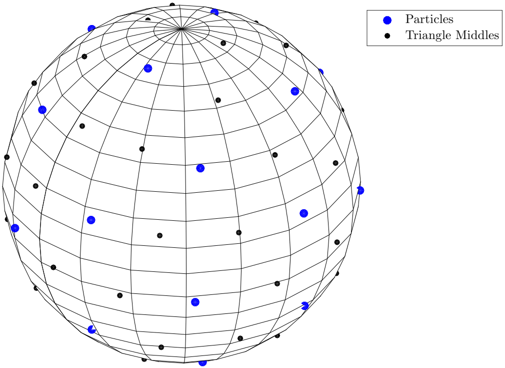


- Implemented mainly in Matlab.
- Start from $N = 4$: tetrahedron.



- 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 $N \rightarrow N+1$.

Removing Redundant Configurations

- Geometrical symmetries!

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- Coordinate-invariant characteristics of a configuration: energy; pairwise distances; pairwise energies...
- Many details will be given in the next talk.

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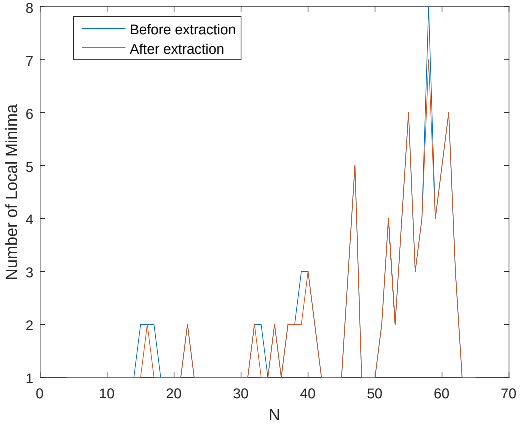
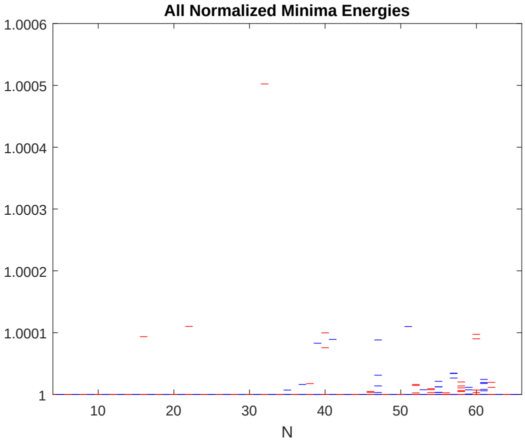
Computational Results: Coulomb Potential, $N \leq 65$

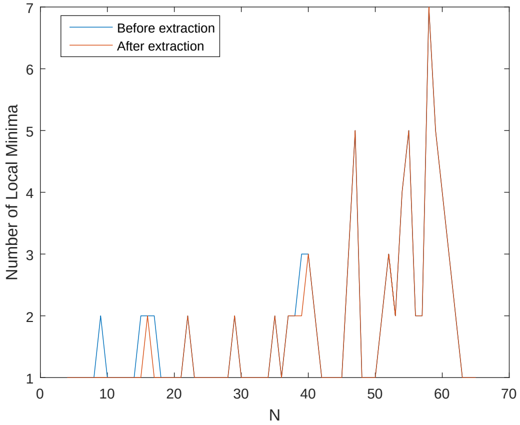


- Number of locally optimal configurations found for the Coulomb potential.



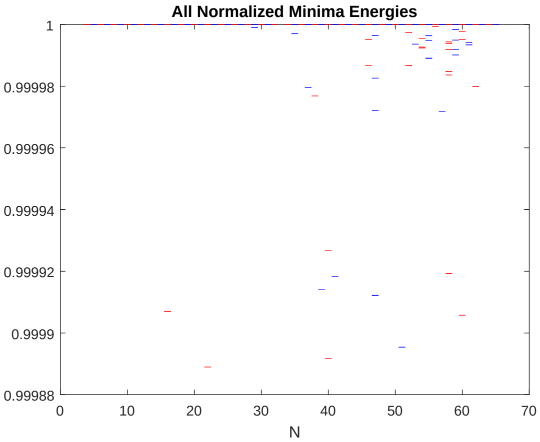
- Relative Coulomb energy spectrum.

Computational Results: Logarithmic Potential, $N \leq 65$



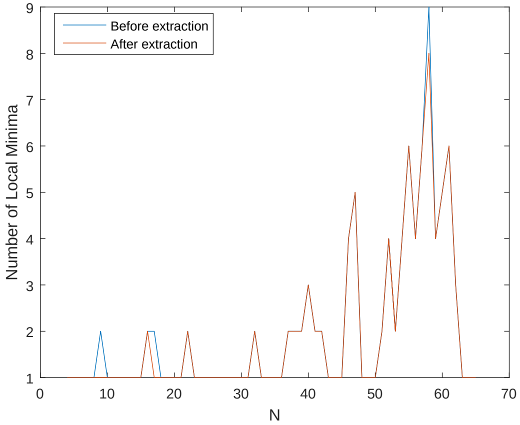
- Number of locally optimal configurations found for the Logarithmic potential.

Computational Results: Logarithmic Potential, $N \leq 65$



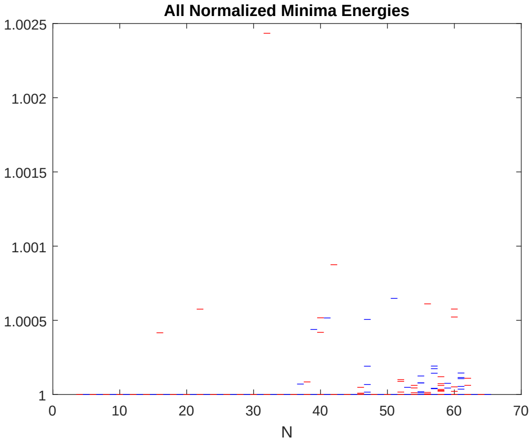
- Relative Logarithmic energy spectrum.

Computational Results: Inverse Square Law Potential, $N \leq 65$

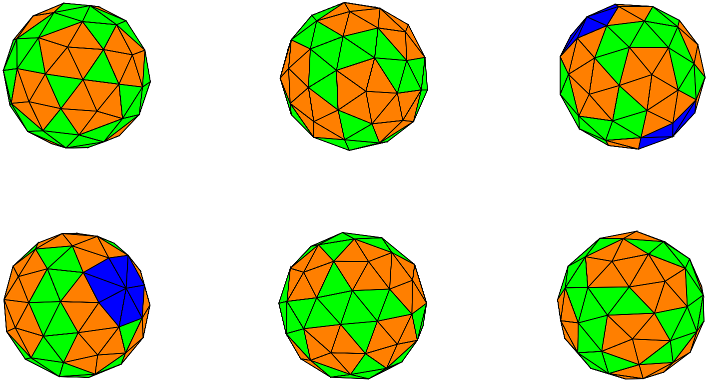


- Number of locally optimal configurations found for the Inverse Square Law potential.

Computational Results: Inverse Square Law Potential, $N \leq 65$



- Relative Inverse Square Law energy spectrum.



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

Outline

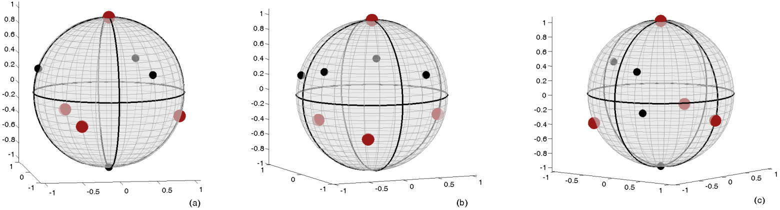
Main findings

- 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?

Some Highlights and Open Problems



- Spherical trap configurations for $2N = 8$ traps of two kinds with radius ratio 10. The global minimum of the average MFPT $\bar{v}$. (b), (c): nearby local minima [*C., Reimer, Ward (2012)*].

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