Energy-Minimizing Arrangements of Repelling Particles on the Sphere: Coulombic and Narrow Escape Potentials

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Motivation & Examples of Applications

Physical Interest

Multiple applications of ordered arrangements of particles on the surface of 3D domains, in particular, the sphere.

- Spherical crystals and crystal defects.
- The Narrow Escape Problem in biology and biochemistry.

Mathematical Interest

Problem of distributing points on a sphere is mathematically rich and has been studied for over 100 years:

- The *Thomson Problem*.
- Distributing points on the hypersphere in higher dimensions.

Specific problem: How can N identical particles be arranged on the unit sphere so as to minimize a potential energy?→ **Local Optimization Problem**

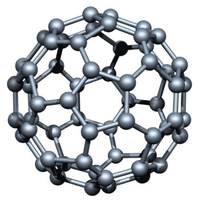

Figure 1: Example of a spherical crystal: a C60 molecule

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The Narrow Escape (NE) Problem and Mean First Passage Time (MFPT)

- The Narrow Escape Problem is concerned with finding the mean time required for a particle undergoing random Brownian motion inside a 2D or 3D domain to escape through small openings on the boundary.
- The time required to escape the domain for the first time is called the Mean First Passage Time (MFPT).
- Transport of molecules, ions, proteins, etc. inside a cell can be modeled by a NE Problem. Particles must escape the cell through a small channel to perform a biological function.
- Minimizing the (average) MFPT minimizes the time required to perform the function.

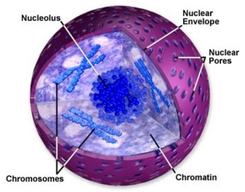

Figure 2: Cell nucleus illustrating small pores through which molecules can escape

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Pairwise Potential Energies

- Functions that depend only on the (scalar) distance between points, $|\mathbf{x}_i - \mathbf{x}_j|$:

$$\mathcal{H} = \sum_{i<j}^{N} h(|\mathbf{x}_i - \mathbf{x}_j|)$$

Coulomb Potential

- Interactions between charged particles.

$$\mathcal{H}_C = \sum_{i<j}^{N} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \tag{1}$$

Logarithmic Potential

- Vortex defects in liquid crystals [1].

$$\mathcal{H}_L = -\sum_{i<j}^{N} \log\left(|\mathbf{x}_i - \mathbf{x}_j|\right)$$

Narrow Escape (NE) Potential

- Asymptotic analysis of the Narrow Escape Problem.

$$\mathcal{H}_{NE} = \mathcal{H}_C + \frac{1}{2}\mathcal{H}_L - \sum_{i<j}^{N} \frac{1}{2}\log\left(2 + |\mathbf{x}_i - \mathbf{x}_j|\right). \tag{2}$$

Formulation of the Narrow Escape Problem

- A particle undergoes Brownian motion in a bounded domain Ω, with small openings (traps) at $\mathbf{x}_i$ on the boundary $\partial\Omega$.
- The remaining parts of the boundary are reflecting.

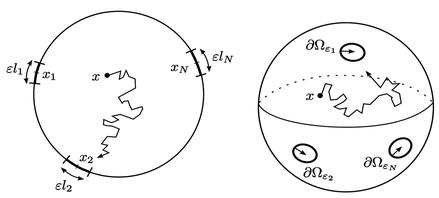


Figure 3: Example domains and particle trajectories [3].

- In the limit of small traps, minimization of the MFPT requires the minimization of the location-dependent Narrow Escape Potential (2).

The Algorithm for Local and Global Optimization

- N particles → $(2N-3)$-dimensional optimization problem in spherical coordinates. For large N, the problem quickly becomes computationally difficult. A fast local optimization routine was developed in C++.

Dynamical system-based optimization algorithm:

1. Start from an initial starting configuration (see below).
2. Compute all tangential forces. On the first iteration only compute the largest of the tangential forces.
3. Increment the particles' positions by an amount proportional to the forces.
4. Project the particle back to the unit sphere by dividing by the norm of position.
5. Compute until the ratio of the largest tangential force to the initial largest tangential force is smaller than the specified tolerance.
6. Compare all locally optimal configurations; choose the putative globally optimal configuration.

Starting Configurations

- Different starting configurations can lead to different locally optimal configurations.
- A systematic method was developed that starts from an N-particle optimal configuration and yields starting configurations for $N+1$ particles.
- For an N-particle configuration, perform the Delaunay triangulation.
- Insert one particle at the center of a triangle to obtain an $N+1$ particle starting configuration.

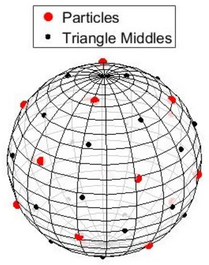


Figure 4: Global minima for the case N=16 showing all 28 triangle centers where the 17th trap can be inserted

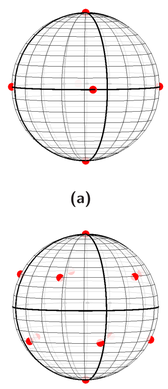
Increasing the Number of Particles. Parallel Computation

- Using the idea for generating starting configurations together with the local optimization algorithm, results for large numbers of particles can be obtained by starting at $N = 4$ and working upwards.

1. Start from the known globally optimal arrangement for $N = 4$: an inscribed tetrahedron.
2. Compute the locations of each triangle center.
3. Insert a particle at a triangle center.
4. Repeat 3) for all triangle centers. Some resulting starting configurations may be geometrically identical due to the high symmetry of the arrangements.
5. For each configurations found in 4), remove all the redundant configurations using an invariant measure, e.g., pairwise distances.
6. For each of the non-redundant configurations, execute the local optimization routine (in parallel).
7. Some of the resulting optimal arrangements will again be geometrically identical. Remove redundant configurations as in 5). Go to 2).

Configuration and Energy Results for the Coulomb Potential

- Few globally optimal configurations have simple/symmetric particle arrangements.
- $N = 5, 6, 7$: one particle at each pole; $N-2$ particles equally spaced on the equator.
- $N = 12$: an inscribed icosahedron, Figure 8.
- Multiple, closely-spaced local energy minima for higher N.



(a) **(b)**

Figure 5: Globally optimal arrangements for (a) N=6 and (b) 12 particles.

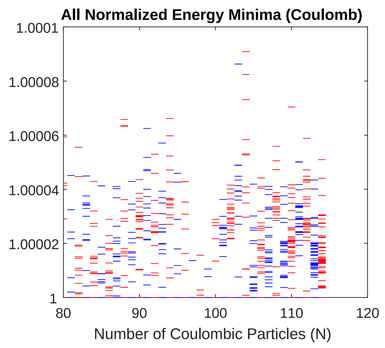


Figure 6: Normalized spectra of local Coulomb energy minima, $80 \leq N \leq 114$

Topological Results for the Coulomb Potential

- Spherical design → Delaunay triangulation.
- The Euler Characteristic: relation between the numbers of vertices (V), edges (E), and faces (F):

$$\boxed{V - E + F = 2.}$$

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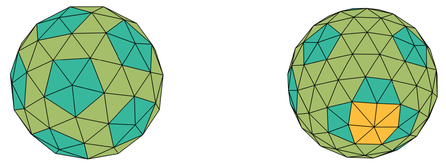
- Tessellation of polygons (cf. soccer ball).
- Fact: spherical arrangements have a defect of 12 (12 pentagons, or 13 pentagons and 1 septagon, etc.)



(a) **(b)**

Figure 7: Defects for the case (a) N=72 with 12 pentagons arranged at the vertices of an icosahedron and (b) N=109 with an irregular arrangement of defects (a **scar**).

- Most configurations have irregularly placed defects but there are 'magic numbers' of particles for which the 12 pentagons form an inscribed icosahedron [2]:

$$N_{mn} = 10(n^2 + m^2 + mn) + 2 \tag{3}$$

Figure 8: Icosahedron

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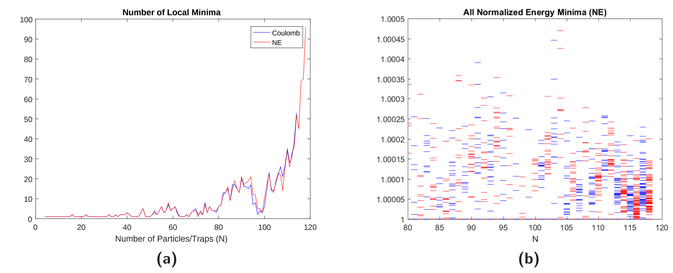
Results for the NE Potential

- The NE and Coulomb potentials have similar numbers of local minima.



(a) **(b)**

- Only the $N = 4, 5, 6, 7, 12, 32$ global minima appear identical.
- Arrangements of defects are often similar.

Local Optimization – Computational Challenges

- Number of local minima increases quickly with N.
- More local minima and higher numbers of particles → more starting configurations.
- Local optimization routine typically performs $> 10^4$ iterations even for $N < 20$; run time of each iteration is $\mathcal{O}(N^2)$.
- Changes in the configuration result in small energy changes, leading to slow convergence in many cases. Local minima have energy spacings as small as 10^{-6} %.
- Occasionally the routine finds 'flat' regions with forces equal to are zero to numerical precision but the configuration is non-optimal. Each configuration is checked by verifying that the Hessian matrix is positive-definite.

Future Work

- Study the topology (arrangement of defects) for different pairwise energies.
- Refine the local optimization algorithm for more exhaustive local minimum analysis.
- Optimizations for larger N.
- Generalize to non-spherical domains.

References

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