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

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.

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 arrangement.
5. For each configuration 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 \( N \).

Topological Results for the Coulomb Potential

- Spherical design → Delaunay triangulation.
- The Euler Characteristic: relation between the numbers of vertices (\( V \)), edges (\( E \)), and faces (\( F \)):
  \[ V - E + F = 2 \]
- Tessellation of polygons (cf. soccer ball).
- Fact: spherical arrangements have a defect of 12 (12 pentagons, or 13 pentagons and 1 septagon, etc.)

Results for the NE Potential

- The NE and Coulomb potentials have similar numbers of local minima.
- 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 \( > 10^6 \) iterations even for \( N < 20 \); run time of each iteration is \( O(N^3) \).
- 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 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


Formulation of the Narrow Escape Problem

- A particle undergoes Brownian motion in a bounded domain \( \Omega \), with small openings (traps) at \( x_i \) on the boundary \( \partial \Omega \).
- The remaining parts of the boundary are reflecting.

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

Figure 2: Cell nucleus illustrating multiple defects.

Figure 3: Example domains and particle trajectories.

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

Figure 6: Normalized spectra of local Coulomb energy minima.

Figure 7: Defects for the case (a) \( N = 72 \) with 12 pentagons arranged at the vertices of an icosahedron and (b) \( N = 100 \) with an irregular arrangement of defects (a soccer ball).

Figure 8: Icosahedron: an inscribed tetrahedron.