The Thomson Problem and Convex Polyhedra

What is the Thomson Problem?

- Originated by the physicist J.J.Thomson in 1904
- Based from the idea of the Plum Pudding atomic model
- To determine the minimum energy configuration of N electrons distributed on the surface of the unit sphere

What is the Thomson Problem?

For a set P of N points randomly distributed on the unit sphere we are required to minimize the total system energy given by

$$E = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j>i}}^{N} \frac{1}{r_{ij}}$$

where r_{ij} is the distance between two points i and j for $\mathrm{i}, \mathrm{j} \in 1..N$.

Monte Carlo Methods and the Metropolis Algorithm

Monte Carlo methods involve generating suitable random numbers in order to obtain numerical results for problems too complex or difficult to solve using analytic methods.

The Metropolis algorithm is one such method where we introduce an accept/reject step determined by the Boltzmann probability of a move.

The Metropolis algorithm requires a symmetric jump distribution which is why the Gaussian and uniform distributions are commonly used.

The Applied Metropolis Algorithm

1. Generate a random set S of N points on the unit sphere

2. Pick a random point of S and generate a new random point from some distribution. Label them S_{old} and S_{new}

3. Compare the energy E of the system for S_{old} with the energy if S_{old} was replaced by S_{new}

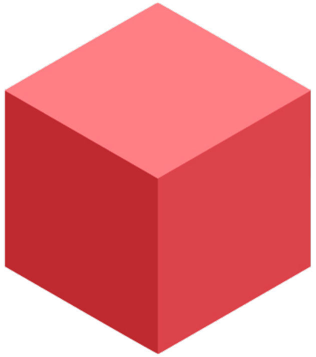
4. If E(S_{old}) > E(S_{new}) then replace S_{old} with S_{new}

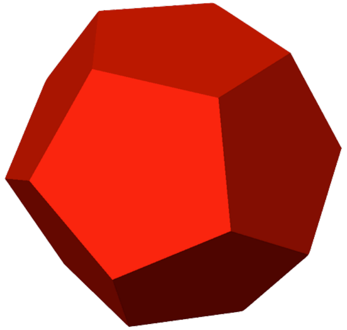
5. If E(S_{old}) < E(S_{new}) then accept the new point S_{new} with probability given by P(S_{new})$=e^{\frac{\Delta E}{kT}}$, where ΔE=E (S_{new})-E(S_{old}), k is the Boltzmann constant and T is the temperature of the system.

6. Repeat steps 2-6 for a given amount of iterations

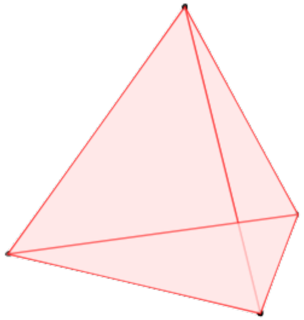
Output Examples

- Iterations I = 100,000
- Temperature $T = 5 * 10^{16}$ K
- Variance $\sigma^2 = 0.0001$

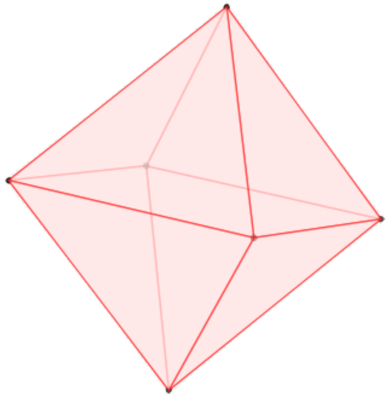




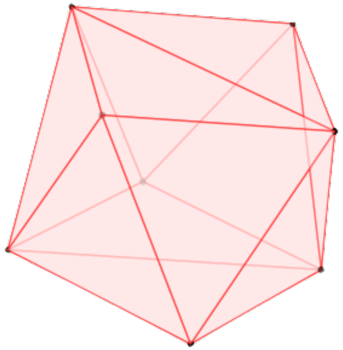
N=4
E =3.674235



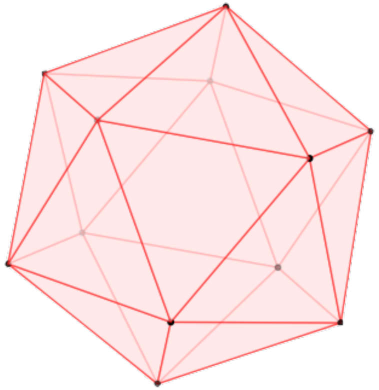
N=6
E=9.985288



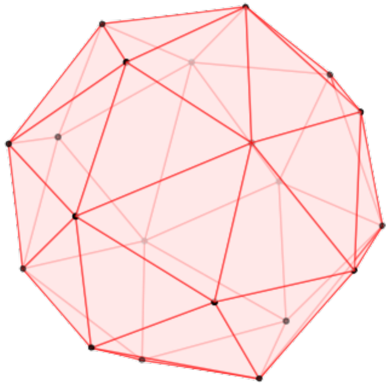
N=8
E=19.675290



N=12
E=49.165261



N=20
E=150.883740

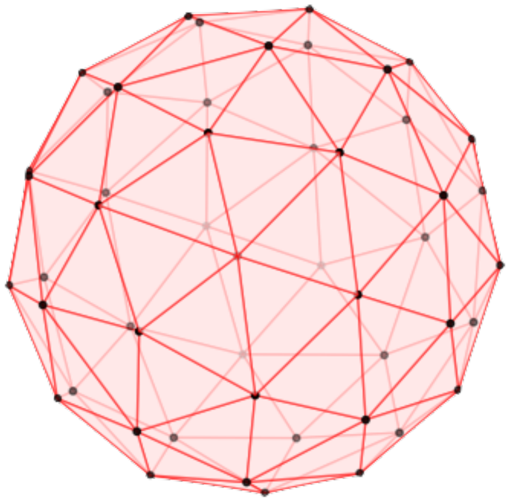


Comparison to Currently Known Minima

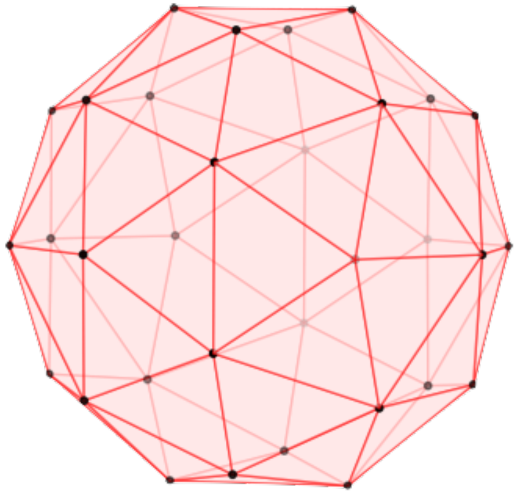
N	Our Energy Result	Current Energy Minima	Difference
4	3.674235	3.674234614	0.000000386
6	9.985288	9.985281374	0.000006626
8	19.675290	19.675287861	0.000002139
12	49.165261	49.165253058	0.000007942
20	150.883740	150.881568334	0.002171666

Courtesy of https://en.wikipedia.org/wiki/Thomson_problem

Large systems and General Trends

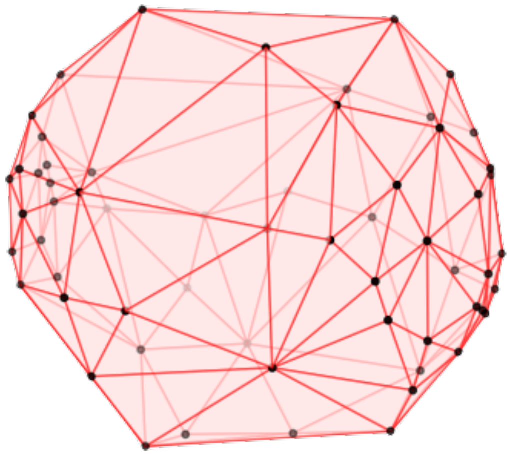


- Hexagonal and pentagonal shapes occur frequently
- Still tendencies towards equilateral triangles if possible
- Small clusters of locally random configurations
- Local minima

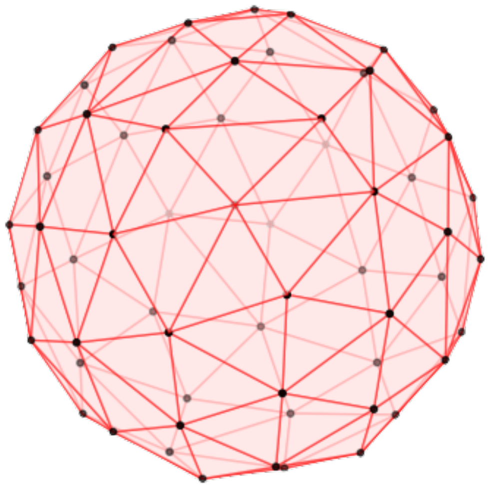


Small Improvements Example

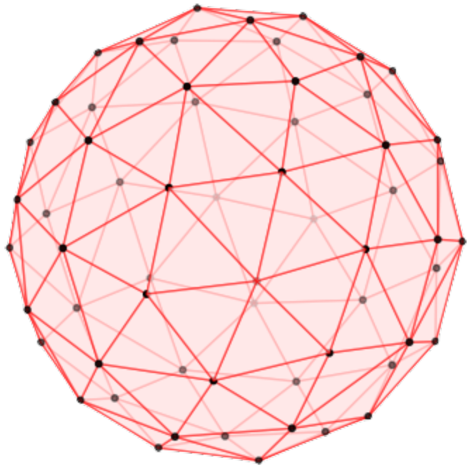
I = 1000
E =1808.092155



I = 10000
E =1545.443486



I=1000000
E =1543.857140



Ongoing Research

- Currently looking at another algorithm, the Wang-Landau algorithm to calculate the density of states of a system
- The Genetic algorithm will also be tested and implemented.