Charge Configuration Optimization with Simulated Annealing

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Abstract—Optimization is an important problem as well in theoretical computer science as in the applied sciences and industrial solutions. But many optimization problems require either computationally expensive brute-force solutions or heuristics developed for just a single problem. Despite the progress in the "divide and conquer" methods or the convex optimization, a general framework for computationally efficient approximated solutions can be an option worth the pursuit for practical applications. Such methods are often obtained by Monte Carlo approach. And here, the concept of simulated annealing relying on the Metropolis algorithm is introduced. It can be used to minimize a functional of many variables as is shown in an example of minimizing the energy of a system of N identical electric charges.

I. Introduction

Optimization is a subject which has been receiving a lot of research throughout the last decades. Solving the optimization problems with brute-force methods often leads to high computational complexity. Thus, approximated solutions with better time efficiency are often worth investigating. Here, following [1], we present a Monte Carlo method for such approximated solutions in form of the simulated annealing with an example of optimization of a system of electric charges.

In the part II, we describe the general problems and approaches to the optimization with the stress on the dual need of both large and small scale effects. Next, in the part III, general Metropolis algorithm is described. Finally, in the part IV, we describe how to use the Metropolis algorithm for optimization by defining the framework of simulated annealing. And in the part V, our experiment is described in detail. In the final part VI, we discuss the results and insights. The code available for reproduction of the results is available at the repository[1].

II. Optimization

The optimization is a process of rearranging the given system in order to minimize a given objective function which is a functional of the system's state. The objective function is often called the loss function.

In the case of the discrete optimization, the direct approach is to check all possible configurations by brute-force. Without any constraints assumed, it leads to the computational complexity of $N!$. On the other hand, in the case of convex optimization, the potential number of configurations goes to the infinity. Additionally, in the continuous optimization problems, one encounters the problem of distinction among local and global minima. Many of the solutions rely on the heuristic methods. Due to that, they are only applicable to a single problem.

The easiest to implement and simultaneously the most computationally expensive methods are trying all possible permutations for discrete problems and generating random configurations for continuous problems. A straightforward upgrade of such solutions is the iterative approach where one generates modifications to the current state by either random changes or based on the gradient of the objective function and accepts only such modifications that lower the value of the loss function. This approach can be very computationally effective, but oftentimes it gets stuck in a local minimum due to only the small-scale optimization. Such a situation requires multiple simulations for different initial configurations, but with no guarantee that the system will not land in the same or other local minima.

Most of the popular problems were answered with efficient solutions till this day by the "divide and conquer" or some gradient-based optimization methods. The "divide and conquer" approach grants both the small-scale and large-scale effects. In case of the continuous optimization, one can never be sure it reaches the global minima, but the modern methods grant some possible extensions to search through most of the space. Despite that, sometimes it might be worth to look for a more computationally efficient, but approximate solution.

III. Metropolis algorithm

In statistical physics, one wants to describe a system of many particles - more than 10^{23}, in such a way that general macroscopic properties of the system can be concluded. A single macro-state of the system corresponding to some macroscopic features as energy or temperature can be realized as many micro-states. The probability of a given configuration (micro-state) C is defined as [2]:

$$P(C) = Z^{-1} \exp(-\beta H(C)), \tag{1}$$

where the function $H(C)$ is the Hamiltonian describing the energy of the system and $\beta = (k_B T)^{-1}$ is the Boltzmann factor depending on temperature.

The Metropolis algorithm is a method basing on Markov chains used in the statistical mechanics to obtain physically relevant configurations as the generation of such multi-dimensional random variables directly from the distribution is impossible. It can be described by the following steps [3]:

1) generate a random configuration C_i,

[1] http://github.com/PGrabinski/SimulationMethods

2) take an element of the state C_i at random and change it to obtain C_t (e.g. flip a random spin),
3) if $E_t - E_i = \Delta E \leq 0$ or a random uniformly sampled number $u \in [0, 1)$ fulfills $u < \exp(-\Delta E/T)$, then set $C_{i+1} = C_t$ accepting the change, otherwise set $C_{i+1} = C_i$,
4) repeat $2-3$ steps N times, where N is the number of elements of the system,

This describes a single Monte Carlo step. At first, n_{therm} of steps are required for thermalization of the system without yielding any reliable knowledge on the system. After the thermalization phase, every Monte Carlo step corresponds to a distinct configuration which can be taken into the considered statistical ensemble.

IV. Simulated annealing

In simulated annealing, we use the analogy to cooling the melted alloys into solids. If one cools liquid metal too quickly, it solidifies into an amorphous structure without any large-scale structure. In case of slow cooling, one can achieve symmetric crystal which shows large-scale organization. Using this analogy requires the introduction of an additional order-related parameter corresponding to the temperature T in the physical picture.

Using this idea, we can minimize any functional of the system state $E(C)$ by the Metropolis algorithm. This approach shows the dual nature similar to the "divide and conquer" methods acting on low-scale due to minimization of the functional $E(C)$ and large-scale duo to the probabilistic acceptances depending on the parameter T. The clue is the slow cooling meaning using a given number n_{MCS} of Monte Carlo Steps per given temperature T_i and slowly lowering the temperature as $T_{i+1} = s \cdot T_i$ where the cooling ratio s is a number close to 1, e.g. $s = 0.9$ or $s = 0.95$.

The challenge in this approach is developing a proper configuration modification generator. For example, in case of the travelling salesman, one could could consider either reversing two neighboring points $(x_i, x_{i+1}) \to (x_{i+1}, x_i)$ or sliding two points along the travel track $(x_i, x_{i+1}) \to (x_{i\pm1}, x_{i\pm1+1})$. These two transformations can bring any given permutation $p(x_1, \ldots, x_N)$, but the number of steps (thermalization) needed for that oftentimes is much higher than the assumed n_{MCS}. This requires at least investigation of the behavior of the system in order to check the thermalization pace, what usually ends in rising the thermalization parameter n_{MCS}. Alternatively, one can introduce some more greedy modification generator either by more significant changes to the configurations or by some heuristic approach in the case where some assumptions can be made.

A more sophisticated approach was proposed in [1]. One can compute an object analogous to the specific heat basing on the variance of the functional being optimized.

$$C_V = \frac{Var(E_T)}{NT^2}$$

Then make the number of steps a function of the specific heat $n_{MCS} = n_{MCS}(C_V)$. This should make the ratio between small-scale and large-scale interactions more effective resulting in a higher chance for finding a better - possibly global- minimum.

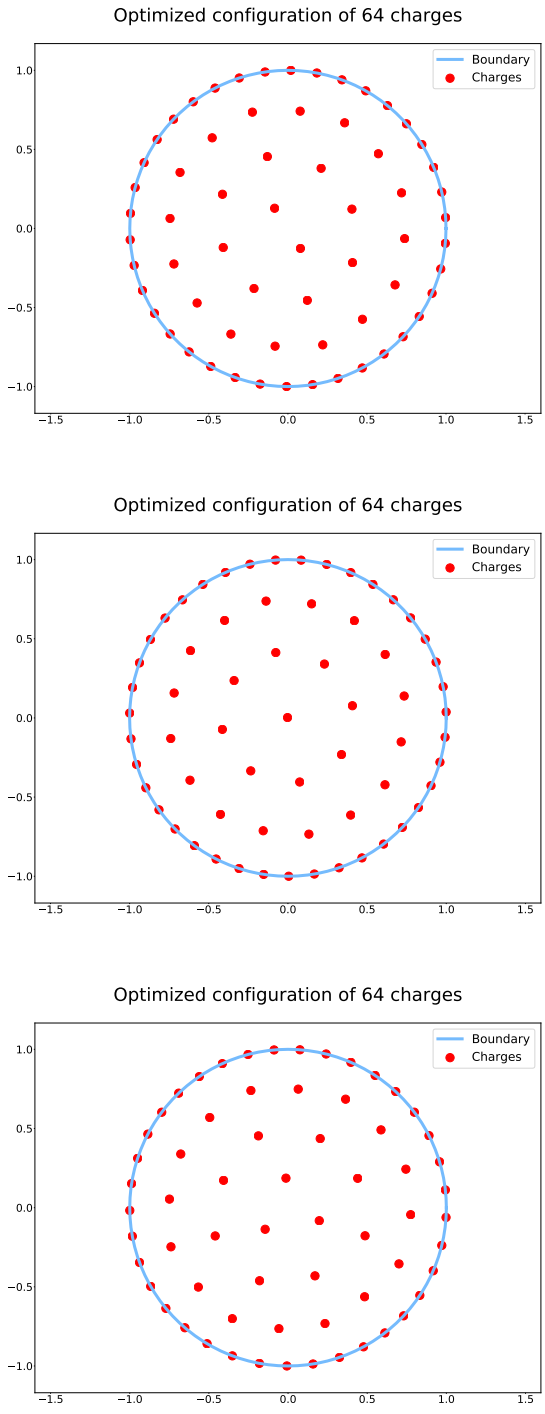


Figure 1. Configurations of the system of $N = 64$ corresponding to local minima. They show emerging structures in the interior of the system space. These structures form new orbits analogous to the charges on the boundary of the system. Top and middle configurations were acquired in the run shown in the figure 5.

Concluding the simulated annealing as an algorithm:

1) generate initial (random) configuration and set initial temperature $T_i = T_{init}$,
2) perform n_{MCS} steps of the Metropolis algorithm with a given functional instead of the Hamiltonian ,
3) cool the system by setting $T_{i+1} = s \cdot T_i$,
4) repeat the steps 2-3 as long as $T_i > T_{final}$.

V. Methods

In our experiment, we use the simulated annealing to minimize the energy of a system of N identical charges in a space bounded by a unit circle. The energy of the system is physically given as:

$$E(C) = \sum_{i,j=1,\ i\neq j}^{N} k\frac{q_i q_j}{r_{ij}}.$$

As we know that the charges are identical and we can set them as $\forall_i q_i = \sqrt{\frac{1}{k}}$. So we get:

$$E(C) = \sum_{i,j=1,\ i\neq j}^{N} \frac{1}{r_{ij}}.$$

Where the r_{ij} is the distance between charges i and j.

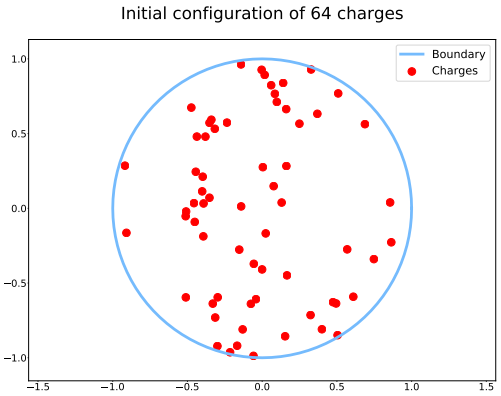


Figure 2. Example of initial random configuration of the system generated in order to obey the boundary limit.

In order to preserve maximal generalization of the solution, we constructed the configuration modification generator as addition of a random uniformly sampled vector $\vec{u} \in (-\frac{\epsilon}{2}, \frac{\epsilon}{2})^2$, where epsilon is a small parameter of order $\epsilon \simeq 10^{-2}$. In case of sampling such a vector $\vec{u}$ that violates the boundary, it is generated repeatedly until an acceptable translation is found.

The experiment was conducted on the following parameter space ($k_B = 1$):

- Initial temperature $T_{init} \in \{1.0, 0.5, 0.1\}$,
- Final temperature $T_{final} = 10^{-5}$,
- Change parameter $\epsilon \in (0.1, 0.5)$,
- Number of charges: $N \in \{10 - 40, 64, 128, 256\}$,
- Cooling ratio $s \in \{0.5, 0.8, 0.9, 0.95, 0.975, 0.98\}$,
- Monte Carlo steps $n_{MCS} \in \{10, 15, 25, 50\}$.

VI. Results and Discussion

It can be seen that the procedure leads to the creation of configurations with symmetric ordered structures as in the figure 1. Such configurations correspond to some energetic minima. The emergent structures are additional orbits. The charges tend to take place not only on the boundary but also inside the system on regularly separated rings.

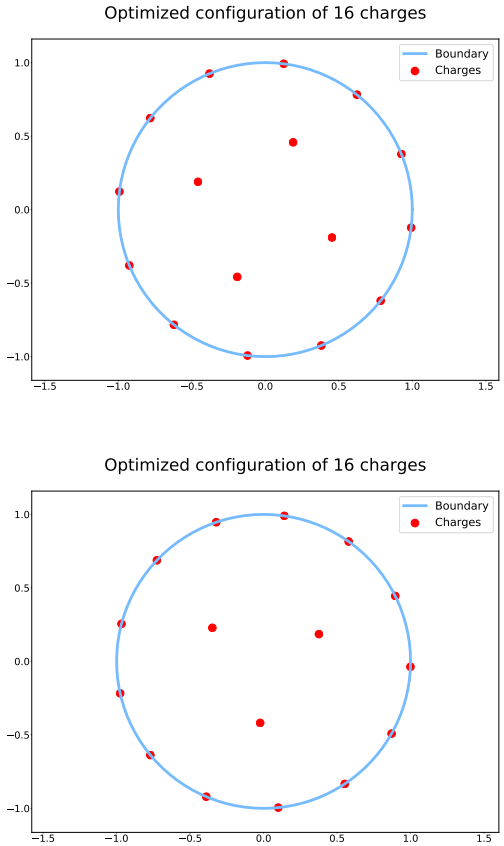


Figure 3. A configuration of 16 charges with 4 charges (top) in the middle of the space corresponding to an alternative local minimum of the energy of 118.94 in contrast to the configuration with 3 charges in the middle (bot) with the energy of 117.46.

The minima can be either local or global - there is no other way to verify it other than finding a better minimum as it was shown in the figure 3.

The main problem of the research when it comes to checking different combinations of parameters is that the system generated in a totally random manner would require a thermalization similar to the one performed in the statistical physics - the phase when observables are not measured as they are not representing the demanded distribution. In this case, the source of the problem is that the random configuration requires so much optimization that combination of low Monte Carlo steps n_{MCS} and cooling ratio $s < 0.9$ yield results without optimization even in the small-scale sense. In case of such parameters initial optimization even basing on iterative improvement

alone without the probabilistic acceptance could be valuable.

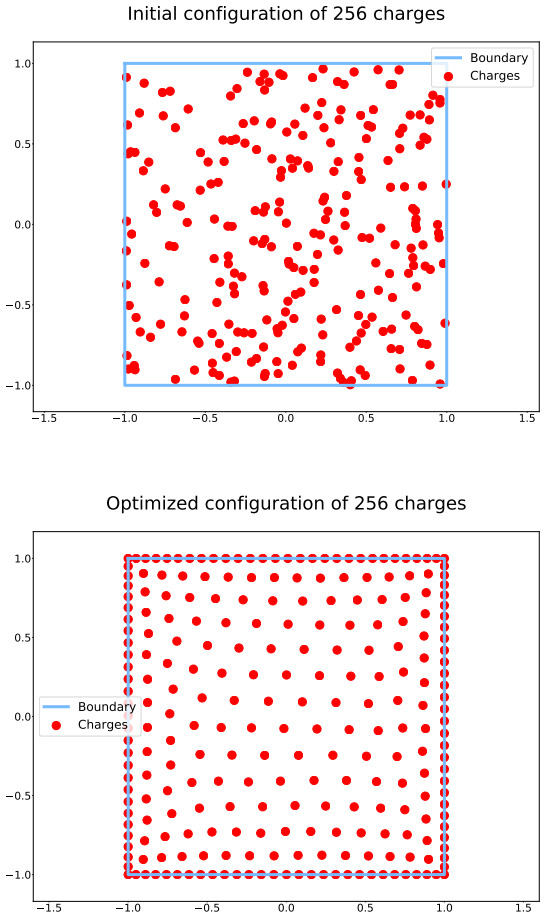


Figure 4. The optimization procedure is easy to generalize to different geometries thanks to the general construction of the modification generation. The initial random configuration (top) and a configuration corresponding to the minimum of energy equal to 39122.17 (mid). The second minimum found was corresponding to the energy of 39124.85. It was not shown due to no naked-eye differences.

We have taken a different approach, performing multiple simulated annealing runs on the same system without randomizing the configuration. It relays on the assumption that the previously found minimum does not require so much small-scale minimization and the disturbance due to induced energy is enough to jump into a region of a different minimum. Proofs that this assumption is valid were shown in the figures.

In the implementation of this method, we have made a trade-off in order to retain as much generalization as possible what was shown in the figure 4. The generalization was traded for computational efficiency. To enable large N computations, it was necessary to develop a method of computing the energy difference between two configurations with complexity $O(N)$ instead of the naive method of calculating whole system energy with complexity $O(N^2)$. The optimization of the system with a square boundary and $N = 256$ charges, $n_{MCS} = 50$, and $s = 0.98$ took several hours of computing. For such a large system and code written in Python, we consider it a good result.

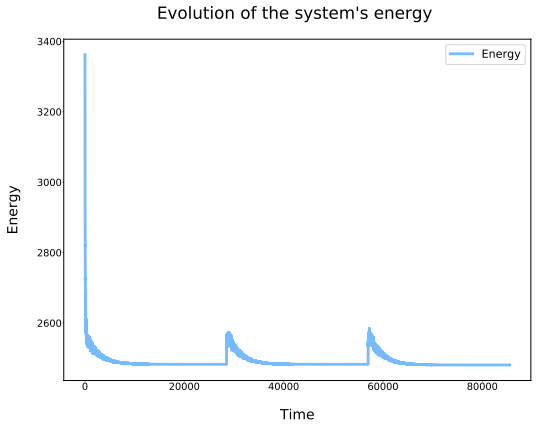


Figure 5. The energy of a system of $N = 64$ charges during three simulated annealing processes. First two minima were constructed with 2 charges inside and were different only by small rotation. The energies of these minima were on the level of 2482.69. The third minimum was at the level of 2480.83 and was constructed with only one charge in the middle as it can be seen in the figure 1.

Also, interesting insight can be taken from the physical perspective. Both of the geometries show expected physical behavior. The circular system corresponds to a charged disk. For a low number of charges, they occupy the boundary of the system. With the rise of the number, we can see that it is also stored homogeneously in the interior of the surface. In the case of the square system, we can see that the density of the charge is higher in the corner. This is equivalent to the fact that the electric field is stronger around the sharp edges of a charged object.

VII. Conclusions

The simulated annealing method is a method definitely easy to implement in the most general way which can solve many problems. As an optimization method, this approach can be very computationally expensive, but in comparison to other methods, it shows satisfactory results. The problem with computational power can be mitigated by introducing more greedy heuristic modification strategies or binding the number n_{MCS} to the behavior of the system. But this investigation is left for future research. In the case of developing a solution to a very repetitive optimization, it could be even reasonable to optimize the average time of optimization by changing the modification generator with evolutionary algorithms, simulated annealing or other methods.

References

[1] Kirkpatrick, Scott, C. Daniel Gelatt, and Mario P. Vecchi. "Optimization by simulated annealing." science 220, no. 4598 (1983): 671-680.
[2] Binder, Kurt, Dieter Heermann, Lyle Roelofs, A. John Mallinckrodt, and Susan McKay. "Monte Carlo simulation in statistical physics." Computers in Physics 7, no. 2 (1993): 156-157.
[3] Oleksy, Czesław, "Lecture Notes on Simulation Methods", University of Wrocław 2019.

VIII. Appendix

Some more interesting example of the simulated annealing are shown in this appendix.

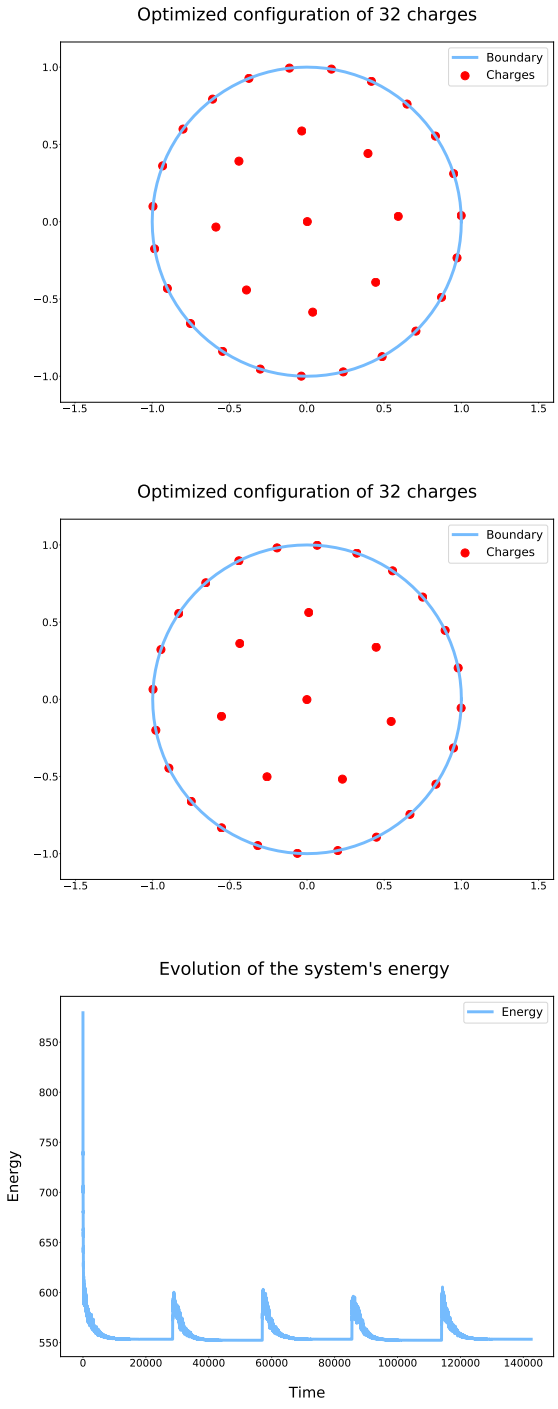


Figure 6. Configurations of the system of $N = 32$ corresponding to local minima. The first minimum (top) with 8 charges on the orbit corresponds to the energy of 553.33. The second minimum (mid) with 7 charges corresponds to the energy of 552.32. The third and the fifth configurations were equivalent up to rations to the one with 8 charges and represented the same energy level as the first one. The fourth minimum was a configuration with 7 charges on the interior orbit with the energy of 552.32. The energy of the system during five simulated annealing processes is shown as the last.

As can be seen in the table I, in a run of 10 consecutive annealing processes for a system with $N = 64$, we have found 3 different minima up to some rotations. The lowest energy corresponds to the configurations no. 8 and 9 with one charge in the middle - zeroth orbit. Later, there are configurations no. 1, 4, and 5 with slightly higher energy with no charges in the middle but, with 2 charges on orbit II and 15 charges on orbit III. Later there is more popular local minimum similar to the previous type, but with one more charge on the orbit III instead of the boundary.

Index	Energy	Or. 0	Or. I	Or. II	Or. III
1	2480.962	0	2	8	15
2	2482.699	0	2	8	16
3	2482.739	0	2	8	16
4	2480.893	0	2	8	15
5	2480.899	0	2	8	15
6	2482.688	0	2	8	16
7	2482.694	0	2	8	16
8	2480.819	1	0	8	16
9	2480.822	1	0	8	16
10	2482.694	0	2	8	16

Table I
Results for 10 minima. Orbit 0 corresponds to the origin of the circle and orbits I-III correspond to the other circles between the boundary and the origin.

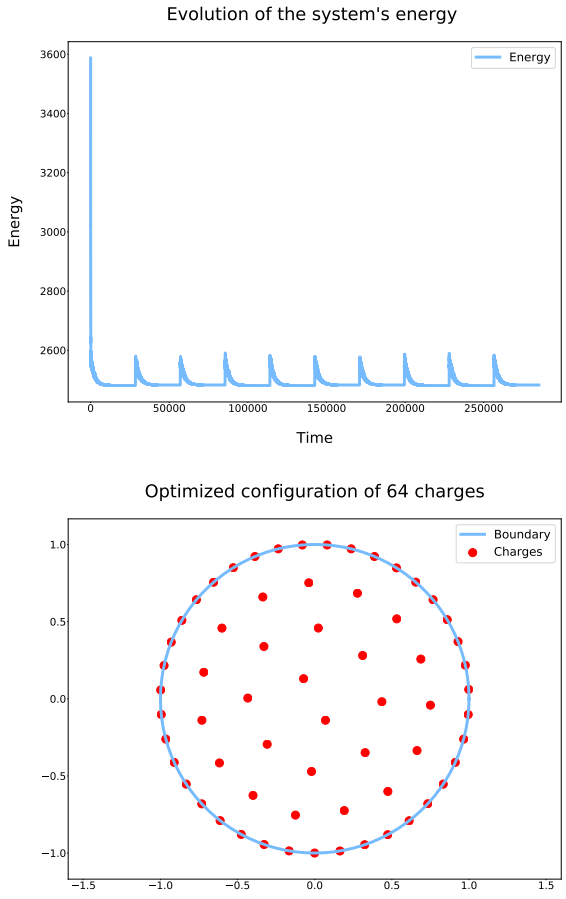
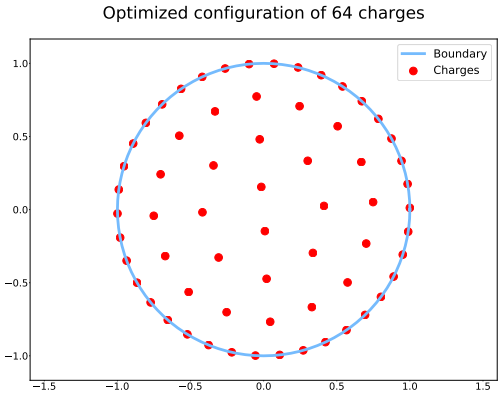
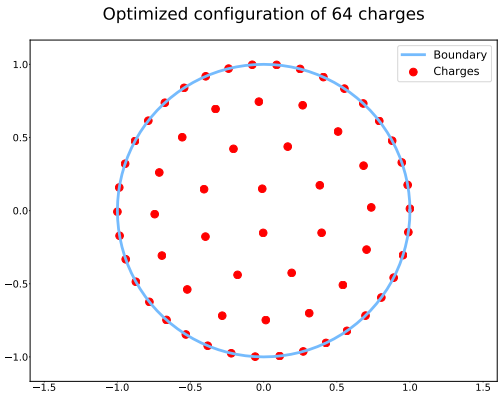
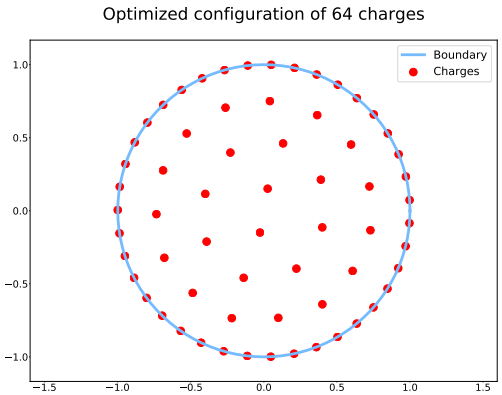


Figure 7. Energy evolution and configuration 1.







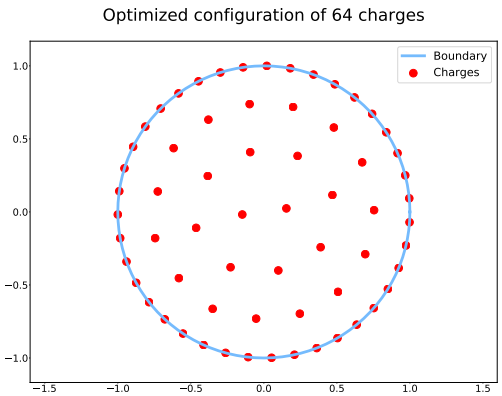
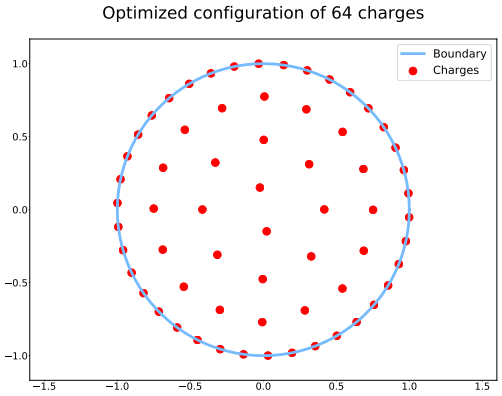
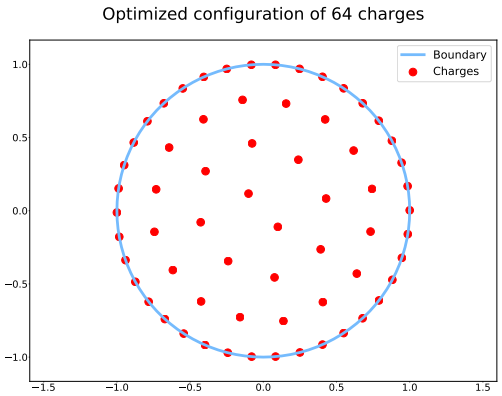
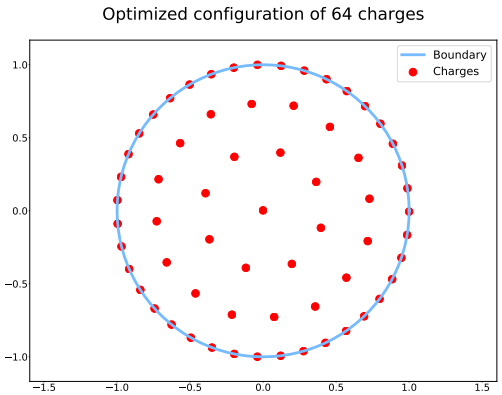


Figure 8. Configurations 2-5.







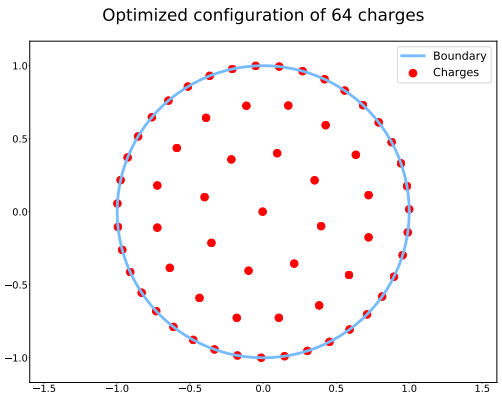


Figure 9. Configurations 6-9.