



Self-Organization of Charged Particles in an Electric Field

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Author's contribution

The sole author designed, analysed, interpreted and prepared the manuscript.

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ABSTRACT

Self-organization in small systems of particles with simple dynamic laws has been simulated. The purpose of this work was to investigate self-organization in small systems of charged particles under the influence of an electric field where we could follow individual particles. There are positively and negatively charged particles. The intention is to look for pattern formation as the system evolves. Three electric fields and the particle-to-particle interactions were utilized to provide the forces. The three electric fields were a constant field, a ramp field, and an oscillatory field. The final system states for various electric fields are presented. For the two kinds of particles simulated, like particles have a repulsive force, while unlike particles have an attractive force. Initially, the particles are randomly distributed in a two dimensional square bounded region, and then allowed to dynamically interact for a number of iterations. Using the inverse square law force, modified at short distances, most cases resulted in equilibrium with the particles of opposite polarity paired up. Since this was a state of equilibrium no more movement occurred. The results of the experiments are presented in graphical format. The main conclusions are that this model can be used to study small dynamic systems, and that the presence of an external electric field does not significantly modify the final configuration but hastens the development of the equilibrium state.

Keywords: *Self-Organization; computer simulation; evolution; dynamics; non-equilibrium; particle-to-particle interaction; cluster formation; electric fields.*

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1. INTRODUCTION

This paper extends the research presented in a previous paper entitled “Self-Organization of Small Systems of Charged Particles with Simple Dynamics [1].” Self-organization in a system is a naturally occurring phenomenon. It can be observed in a number of different situations [1-5]. It can often occur in systems with no external or internal control. Only the internal forces guide the evolution of the system. Self-organization can also occur in non-linear dynamical systems. Self-organization has been addressed in many ways. Most of the approaches are based on a statistical-mathematical framework. One popular approach is referred to as Multi-Agent Systems. This is a Bayesian statistical approach [6]. Another approach is Group Method of Self-Organization Techniques in Modeling [7]. These methods have the advantage of being able to handle a large group of particles or entities and complex dynamics. The work presented here is a numerical simulation study of self-organization, and the dynamics provided by the simple inverse square force law and an external electric field (E-field). Our method has an advantage over the statistical methods of being able to follow an individual particle or a small group of particles throughout the evolution of the system. Our emphasis is on the simplicity of the system and the resulting outcome using simple dynamics. Our approach has already been used to study the propagation of infectious diseases [8] and to follow the migration across a common boundary [9]. These two papers used the same basic

framework as this paper with some modifications. Some parts of these papers and some of [1] are repeated here to make this paper as clear and complete as possible. It appears that this approach could be used in any situation in which using a small number of particles are enough to give some insight into the system evolution. It is necessary that the forces can be easily defined and coded. This paper reports the effects on the evolution and organization of a set of charged particles with external E-fields present. The systems described here have two kinds or types of particles. Within each type the particles are identical except for their initial location. The two types of particles are similar, but the two types have different interaction strength. Numerically the strengths are the same but have opposite signs. Additionally, one type of the particles was less responsive to force than the particles of the other type. Hence, with some changes the two types could be designed differently, but the interactions used here within and outside the type are simple to describe. The dynamics are determined by a set of rules that the particles follow. The more responsive particles are referred to as e-particles and have a negative strength. The less responsive particles are referred to as p-particles and have a positive strength. In all that follows the system was contained in a square of size 512 by 512. At initiation the particles are located by randomly placing them in the square. A sample initial distribution for a system with 100 particles is shown in Fig. 1.

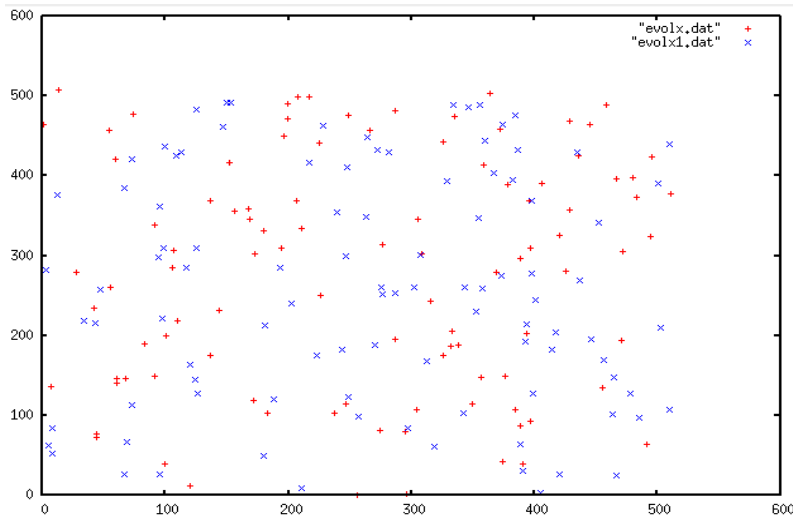


Fig. 1. An initial distribution for 100 particles of e and p types; Red “+” denotes e-particles and blue “x” denote p-particles

There were three external fields applied. The first was a constant field over the particle domain, the second field was a linearly increasing field over the particles and the third was a field oscillatory over the domain. The total field over the particles was the vector resultant of the fields. Results are given for the fields applied separately and collectively. That is the results are given for the fields applied individually, in pairs, or all three. In addition, results are given for no applied field for comparison purposes. The system evolves to a frozen and cold state, but may still provide insight into some systems. Thus the results of the movement can be studied and analyzed. Our outlook is that we have created a tool that can be used to study self-organization for a number of different scenarios. The program collects statistics that can be used to study the system evolution. Two sets of results are given one is for 100 particles of each type and secondly for 500 particles of each type.

One of the interesting parameters calculated was the system temperature. The system temperature was taken to be the velocity squared. The final configuration after a suitable number of iterations was taken showed that most of the particles paired up in an equilibrium condition. At this point there was no unbalanced force and all motion stopped.

The rest of this paper is organized as follows. In Section 2 the method and the program are described. Section 3 gives the results. Section 4 gives some discussion, and the conclusions, and potential future work.

2. METHODS

The method used here was computer simulation. The program, with some minor modification was the same program used in [1]. Much of the description given there is repeated here so this work is complete. The program was constructed in functional form using the c programming language. Specifically, the gcc compiler running under the Debian version of Linux was used. For this work, the main modification of the existing program was to add the forces on the particles due to the presence of an E-field. The programming was straight forward, and no programming tricks or shortcuts were used. This makes the program easy to follow and modify as needed. The functional form makes it relatively easy to add or delete features. However, there is a lot of bookkeeping involved in calculating the forces and managing the particle dynamics. A

great deal of care was taken and a lot of checking was done to make as sure as possible that the program was correct.

2.1 The Forces

There are two types of forces. The internal forces of the inverse square law and the forces due to the presence of the E-field.

2.1.1 The Inverse square law forces

As stated earlier, it was assumed there exists two kinds of particles with simple dynamics and they are referred to as e and p- particles. Every particle interacts with every other particle. Each particle was assigned a force strength. For this experiment the force strength was the same for all particles with value 25. The particles interact such that the force on particle i by particle j was

$$f_{ij} = S_i S_j / d_{ij}^2, \quad (1)$$

where s_i and S_j was the strengths of particles i and j and d_{ij}^2 was the square of the distance between particle i and particle j as shown in Fig. 2. The force is either repulsive or attractive and acts along the line between the two particles. If e represents one type of particle and p represents the other type then the e-e and p-p interactions are repulsive. The e-p and p-e interactions are attractive.

2.1.2 The E-field forces

The external forces were those from the E-field. The direction of the E-field was in the positive x direction. There were three electric fields used. The parameters to define the strength of the E-fields are e_0 , e_1 , and e_2 . The first was a constant field, the second was a ramp and the third was an oscillatory field. That is we used $e_0=c$ for the constant field. For the ramp field, we used $e_1x/512$ where x is the location of a particle on the x-axis. For the oscillatory field we used $e_2\sin(2\pi 15t + 2\pi 15x/512)$. Two of the fields are shown in Fig. 3 and the force at location at $x=510$ with all fields applied is shown in Fig. 4. The force applied to a particle at position x was given by the strength of the electric field at that location times the strength of the particle. That is, the force on the particle is eS where e is the magnitude of the E-field and S is the strength of the particle. For positively charged particles S

was positive and for negative charged particles S was negative. That is, if the E -field acted alone the positive particles moved in the positive x direction, and negative charged particles moved in the negative x direction.

2.2 The Dynamics

As stated earlier, the dynamics are governed by a set of forces between each pair of particles i and j by Eq.(1), and the forces on each particle by the external E -field. In all cases considered here the distance between the particles is the Euclidean measure as shown in Fig. 2.

$$\begin{aligned} dx &= x_j - x_i \\ dy &= y_j - y_i \\ d_{ij} &= \sqrt{dx^2 + dy^2} \end{aligned}$$

The arrow shows the direction of a repulsive force. The simulation proceeds at discrete intervals according to the dynamics equation $d = d_0 + f \delta t$ where d_0 was the x or y coordinate before an iteration step, d was the coordinate after an iteration step, δt was the size of the iteration step, which was either δx or δy depending on whether x or y was being updated. f was the total force acting on the particle in the x or y direction. The p - particles were assumed to be less responsive to a force

than the e -particles. This was implemented by making the response to the applied force a number of times smaller for the p -particles than for the e - particles. The δt for e -particles was 0.01 and for the p - particles was usually 100 to 1000 times smaller.

The implementation of the dynamics deserves some further explanation. Employing these dynamics bears a significant similarity to integrating the equations of motion for the inverse square law force. When two particles are far apart the force is small because of the distance squared in the denominator. Hence, when the distance to be moved by the particles is small a relatively large step size could be used. As the particles get closer together the force naturally increases. At a certain distance between an e - p pair, called the critical distance, d_c , the distance to be moved was equal to the distance of separation. This distance was

$$d_c^3 = S_i S_j \delta t. \tag{2}$$

If the distance between the particles was smaller than d_c the two particles would pass each other when moved via the dynamics. It was necessary to shorten the step size to prevent this. This was accomplished by moving the particle 0.1 of d , the distance between the particles. The distance was calculated and the particles were moved accordingly.

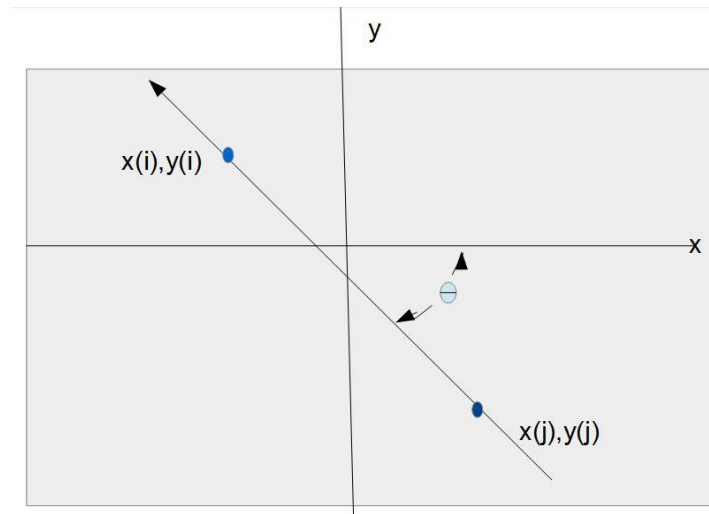


Fig.2 Graphical description of distance from $(x(i),y(i))$ to $(x(j),y(j))$; This also shows the force on particle i by particle j if the force is repulsive; If the force were attractive the arrow would point in the opposite direction; $\Pi-\theta$ is the angle between the force and the x -axis

2.3 The Simulation

The simulation proceeded as follows:

- a. n particles of each type were created and placed at random in a 512 by 512 square.
- b. The strength of each particle was assigned. All of the particles have the same strength of $S=25$. S was either positive or negative.
- c. The vector distance between every pair of particles was calculated.
- d. The net force on each particle was determined by vectorially adding all of the forces from the other particles and the E-field.
- e. The dynamics were then applied to obtain the new position of each particle.
- f. With the new locations known the process starting at step c was iterated. The process was repeated for a given number of iterations.

In looking for a set of operating parameters, we found that our first choice of S and δt were too large. The effect of these choices was that a particle moved too far at an iteration. The particles were hitting the edge of the square too soon and too often. When a particle left the square it was re-injected to keep the number of particles constant. The rule was that if a particle left the square on an iteration it was injected

back into the square at a random location. If this happened too frequently the chance of reaching equilibrium was unlikely. It was found that a strength S of 25 was usable and δx and δy were both 0.01 for e-particles and 0.001 for p-particles. We believe other values could be chosen with successful results.

To find useable strengths for the three E-fields the following calculations were done. On a square with side of length one the average distance between two points chosen at random is approximately 0.52. Then for a square with side of 512 the average distance is approximately 266. A particle does not interact with itself, so there is one particle of opposite sign to interact with a given particle if all are considered to be at the average distance. If the strength of the E-field is one on a particle and the force from another particle is the same then from Eq. (1) the two forces have the same value of 25. This means that if the distance between the two particles was larger than 25 the E-field force was the larger and if the distance was less than 25 the particle-to-particle force was the larger. Since we wanted to look at effects for relatively small E-fields, this seemed to be an acceptable range for the forces. So for the 100 particle cases $e_0=e_1=e_2=1$ was used. For the 500 particle case $e_0=e_1=e_2=25$ was used. In this case the larger force was from the E-field if d is larger than one. The particle-to-particle force was the larger for d less than 1.

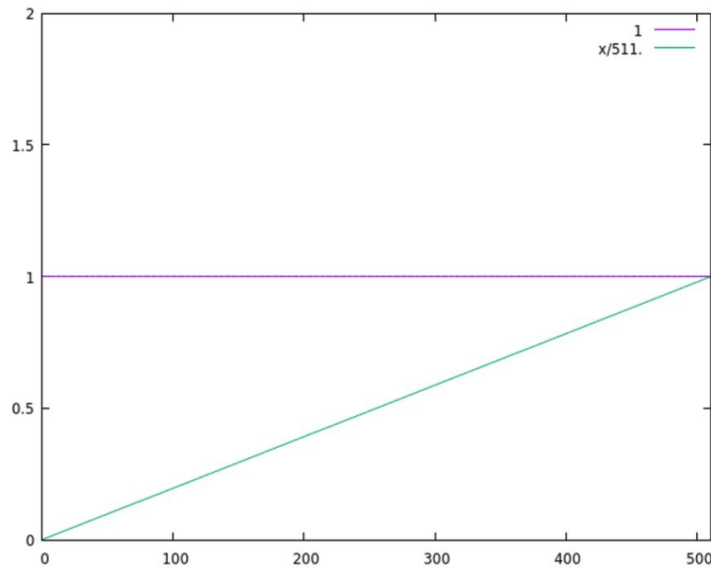


Fig.3 The External Electric Fields. The purple line represents the constant field; The green line represents the ramp field; For both fields the direction of the field was in the positive x direction

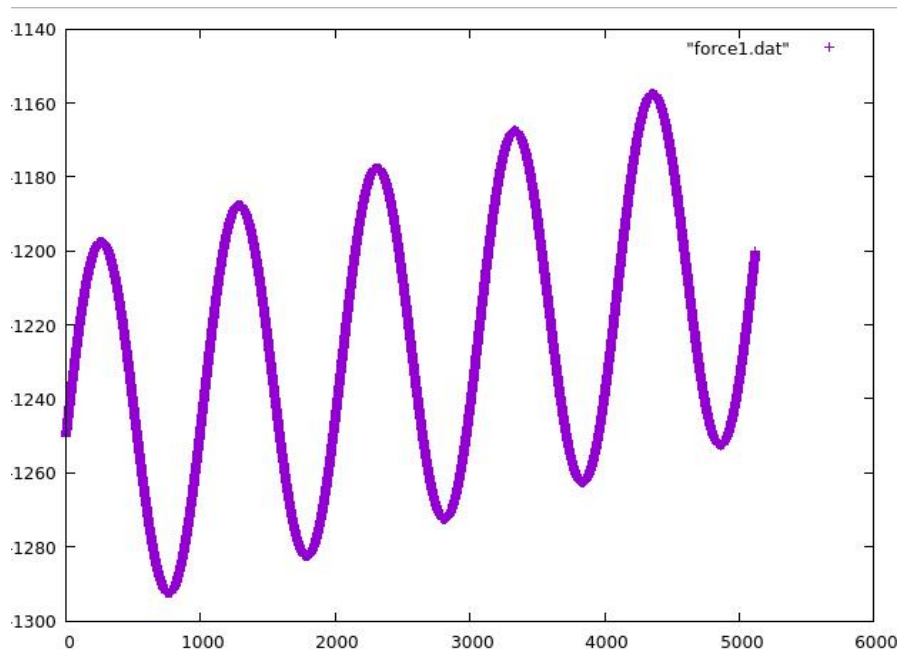


Fig. 4. The total force applied to a particle at location $x=510$ when all three fields are applied

3. RESULTS

Results were obtained for 100 and 500 particles.

The results obtained were for the three kinds of E-fields as described above. The simulations were performed for all combinations of the fields for the 100 particle cases. Only one result was taken for the 500 particle case, and this was with all of the E-fields in place with a magnitude of 25. All simulations were for 1 million iterations. The 500 particle case was for 1 million iterations and took approximately three days (72 hours) to complete.

In some of the figures for the temperature the maximum value of the abscissa is 500,000. The total number of iterations was 1,000,000. This was achieved using two runs of the program. The program writes out the final values of the particle coordinates, and these values can be read at the next run of the program. The number of iterations was written at the end of the second run as 500,000. All of the results presented here are for 1,000,000 iterations.

The results of the simulations are given in graphical form. One graph for each simulation gives the final particle configuration in the 512 by 512 square. For the initial configuration we rely on Fig.1, because all original positions are

random and are very similar. The second graph for each simulation displays the system temperature. In most cases shows the final temperature was at or near zero. This indicated the system had reached an equilibrium condition. The simulations were labeled by the E-field strengths e_0 , e_1 , e_2 . The ones presented here for the 100 particle case are 000, 100, 010, 001, 110, 101, 011, and 111. For the 500 particle simulation only 111 was carried out.

The final state graph appears to show that the particles are mostly paired up. At initiation we have a certain temperature. The temperature for a pair of particles varied based on the distance between the particles and the value of the E-field. The final configuration in most cases was such that the particles are coincident pairs. Hence, at this point there are no unbalanced forces and the temperature is zero. At the beginning the particles are uniformly distributed, the forces are large and so is the temperature.

The program was run many times for 2, 10, 16, and 100 particles of each type and once for the 500 particle case. We ran the 2 particle case as well as the 10 particle cases to gain confidence that the program was correct. To further gain confidence that the code was correct hand calculations were performed. The hand calculations found the force and movement of

several particles. These values were compared to values printed out from the code. These checks were done at various times during the development of the code. We think these checks verify the code as far as is humanly possible. In the two particle simulation there were two particles of each type, i.e. two e-particles and two p-particles. There was convergence to two pairs. With the parameters used here the number of iterations to convergence was about 3 million. The result was a pairing of the particles with one e and one p-particle in each cluster. The temperature was at a minimum, and there was no movement by an e or p-particle. Further, any try at movement by a particle would be corrected on the next iteration by the attractive forces between the e and p-particles. After convergence a number of iterations confirmed no further movement took place. The results for the 10 particles showed a one-to-one pairing of e and p-particles after about 5 million iterations. Also the e and p-particles were coincident at the final configuration for the 16 particle simulation. Since the results for the 10 particle, 16 particle and 100 particle models were very similar the discussion will be on the 100 and 500 particle case. For the 100 particles of a type case we are showing the final configuration. Even after a large number of iterations a one-to-one pairing does not occur in all cases with the parameters used. At the end,

some of the p-particles have captured two e-particles leaving some of the e-particles unpaired. The configuration was stuck in a local minimum. Further changes were impossible unless something occurred to break the deadlock. However, all real systems have some inherent noise. In [1] to break the deadlock a test was used to find if two e-particles were within a check distance of 0.001. If this test was passed the two e-particles were moved a random distance and the iterations continued. The distance moved was randomly distributed over -1.0 to 1.0. This was sufficient to break the deadlock and the system was free to seek another minimum in the temperature. Introduction of the noise as allows the system to evolve to a pairing of all e and p-particles. This process was not used in this paper as we regarded it as unnecessary for our results presented here. The collection of two e-particles by one p-particle is interesting though. There was some evidence of a collection of particles occurring. However, as mentioned above this configuration was a stable equilibrium, and after many more iterations the temperature remains unchanged. This system evolved to a cold and frozen system, and it is not very interesting from that point of view. However, there may be situations where equilibrium is a desired outcome.

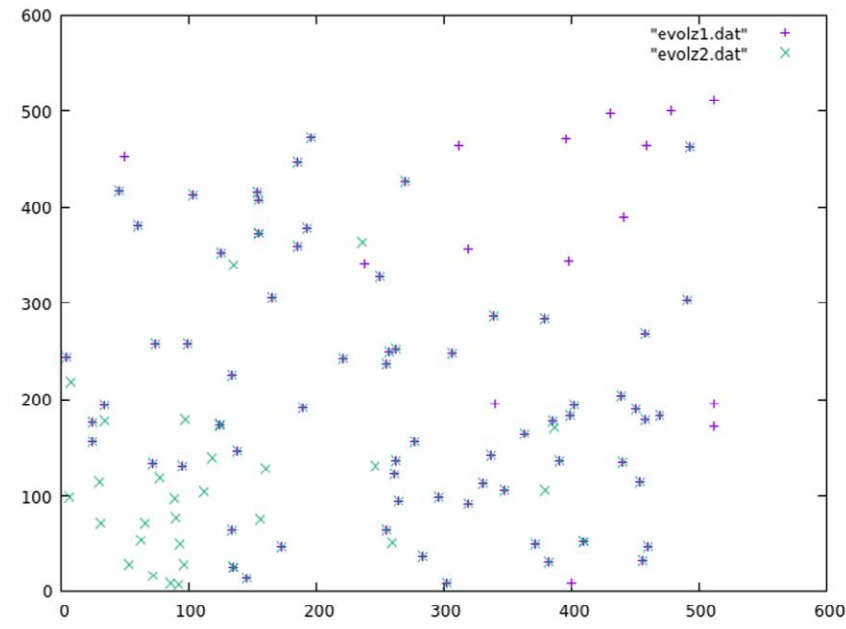


Fig.5. Final configuration 100 particle for field 000; Red “+” denotes e-particles and green “x” denotes p-particles; Mostly paired up, but still some movement as can be seen in the temperature plot of Fig. 6

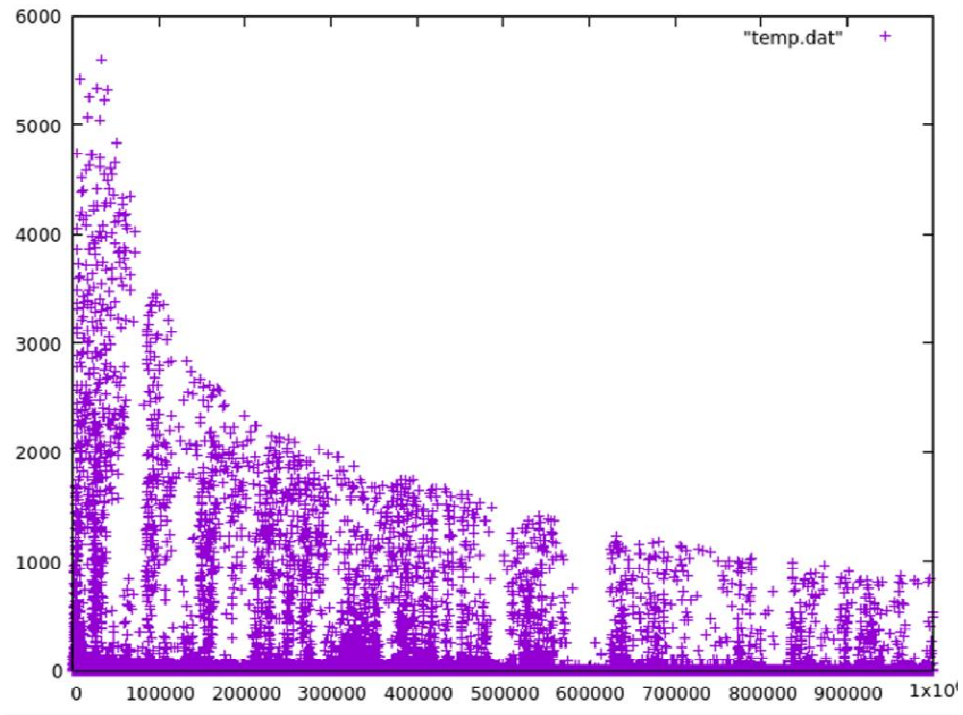


Fig. 6. The temperature evolution for 100 particles with field 000

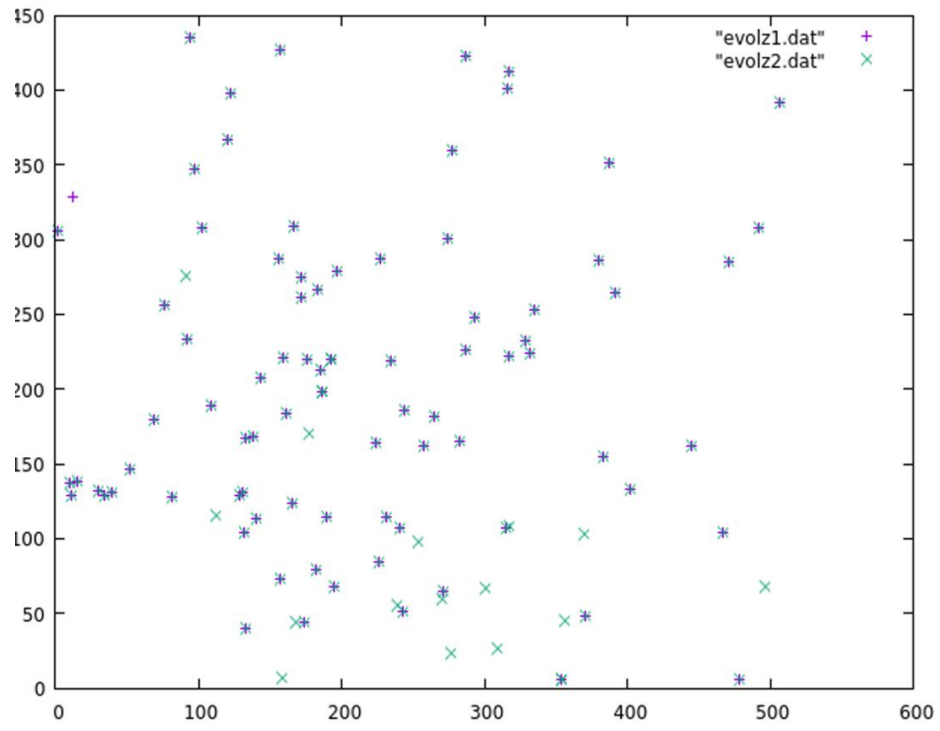


Fig. 7. The final configuration for the 100 particle case with field 100; Red “+” denotes e-particles and green “x” denotes p-particles; Mostly all paired up after just 500,000 iterations

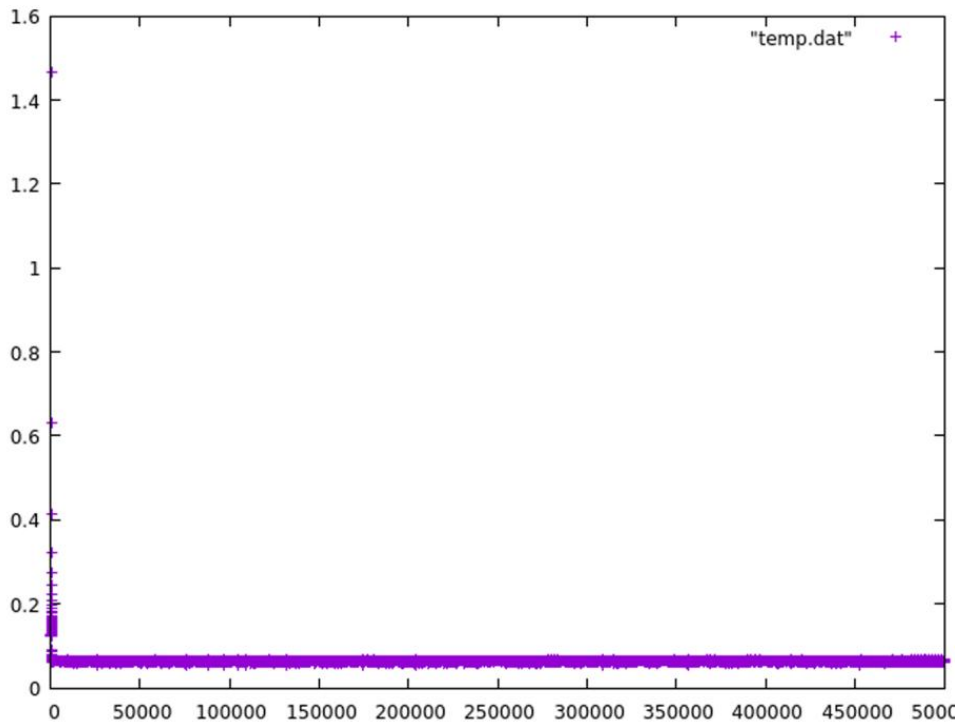


Fig. 8. The temperature for the 100 particle case with field 100

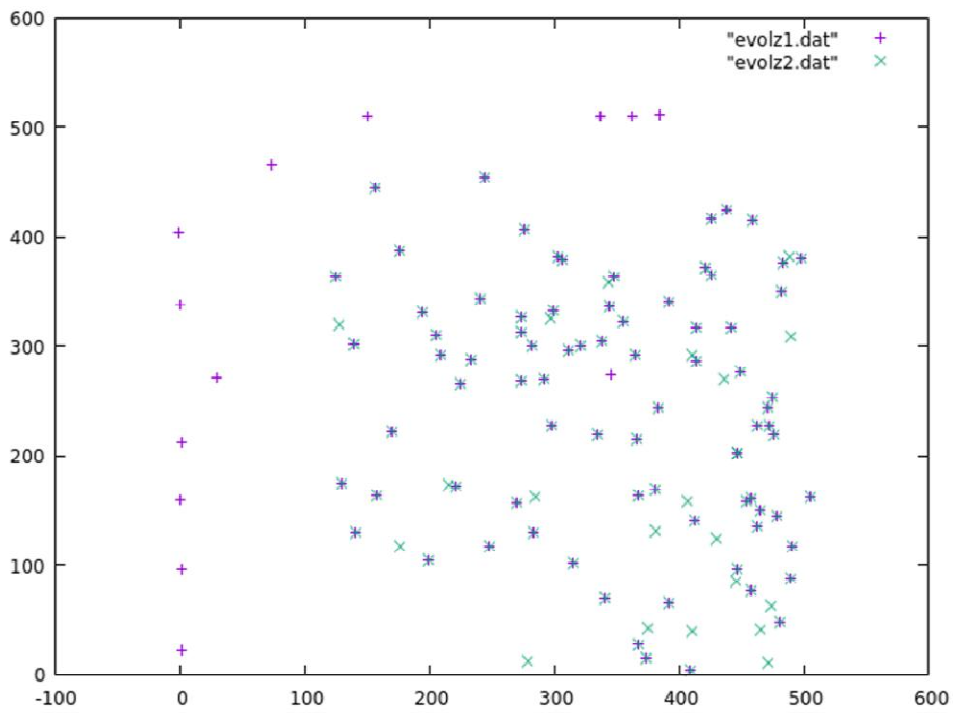


Fig. 9. Final configuration for 100 particles and with field 010; Red “+” denotes e-particles and green “x” denotes p-particles; Mostly paired up, but showing definite preference for e-particles to the left, and p-particles to the right

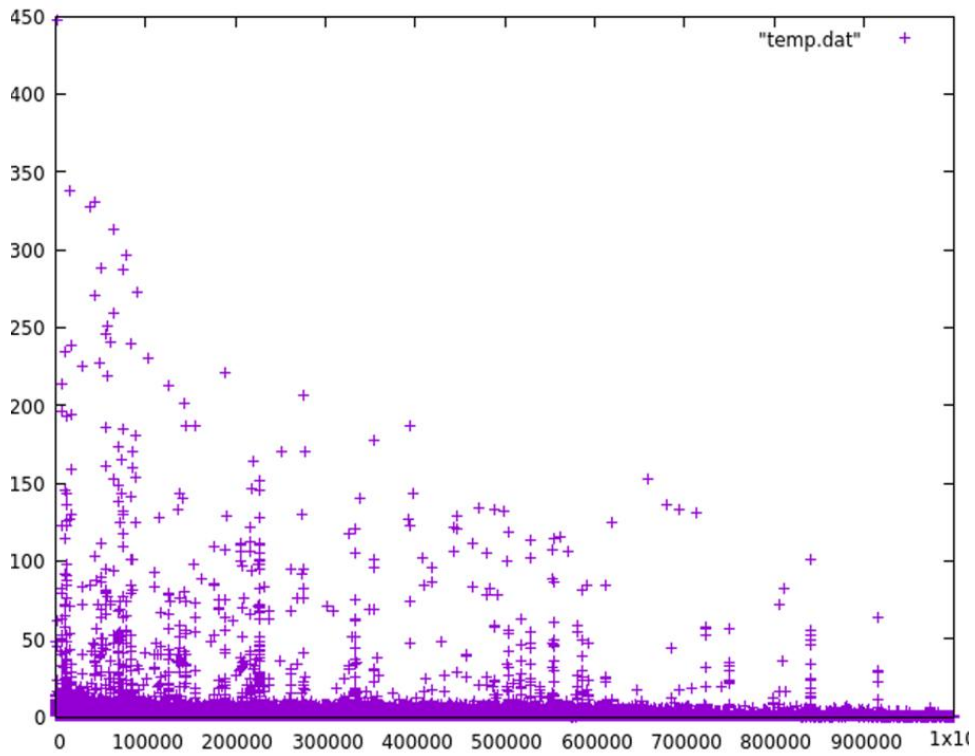


Fig. 10. The temperature for 100 particles with field 010

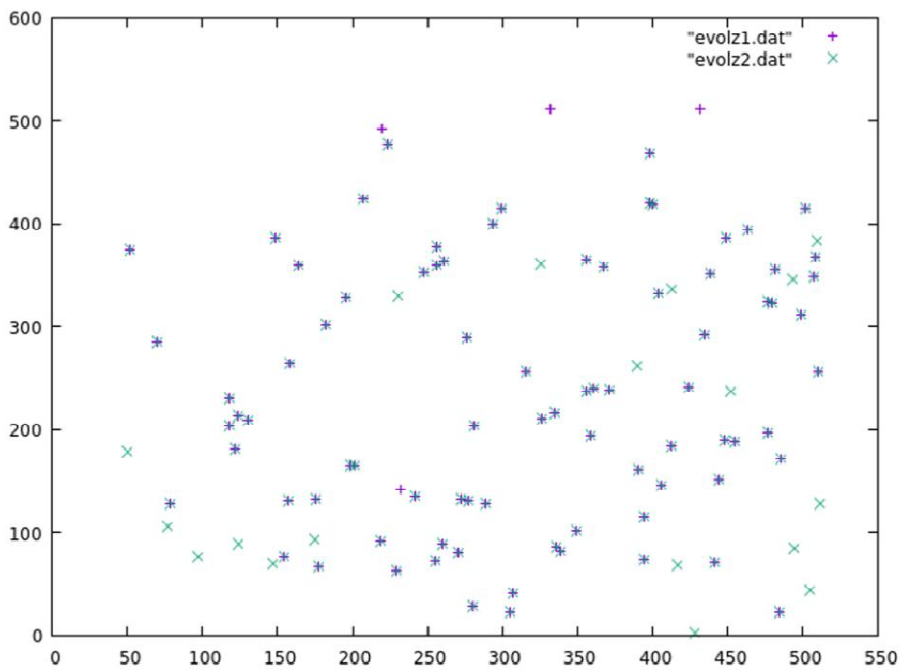


Fig. 11. The final configuration for 100 particles with field 001; Red "+" denotes e-particles and green "x" denotes p-particles; Mostly paired up; Temperature at zero after 500,000 iterations as displayed in Fig. 12

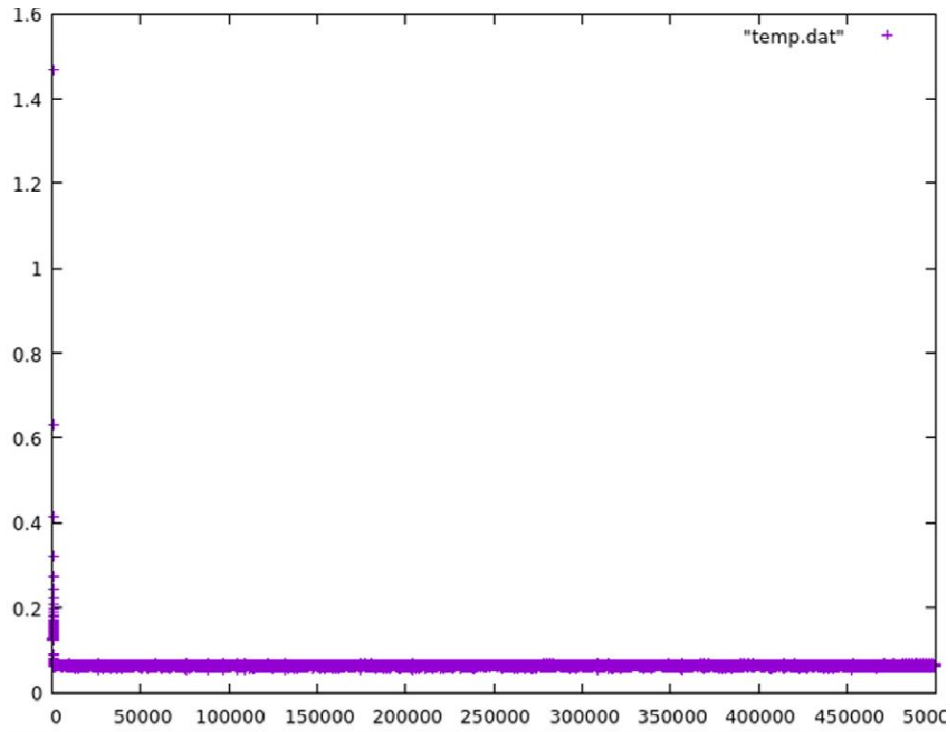


Fig. 12. The temperature for 100 particles with field 001

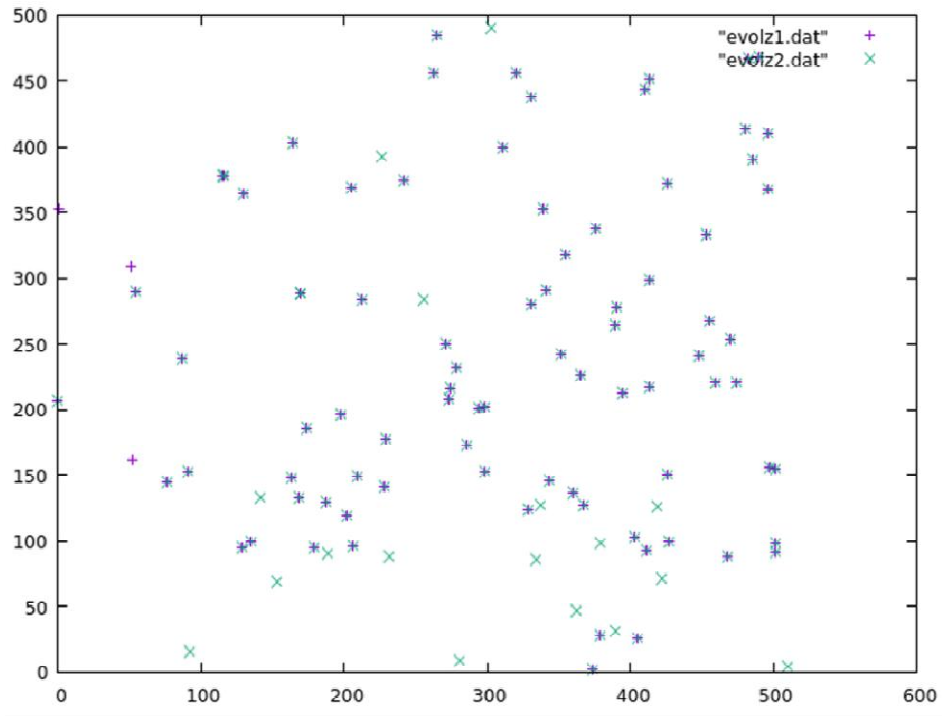


Fig. 13. The final configuration for 100 particles with fields 110; Red “+” denotes e-particles and green “x” denotes p-particles; Mostly paired up; Some preference for e-particles to the left, and p-particles to the right; Temperature at zero after 500,000 iterations

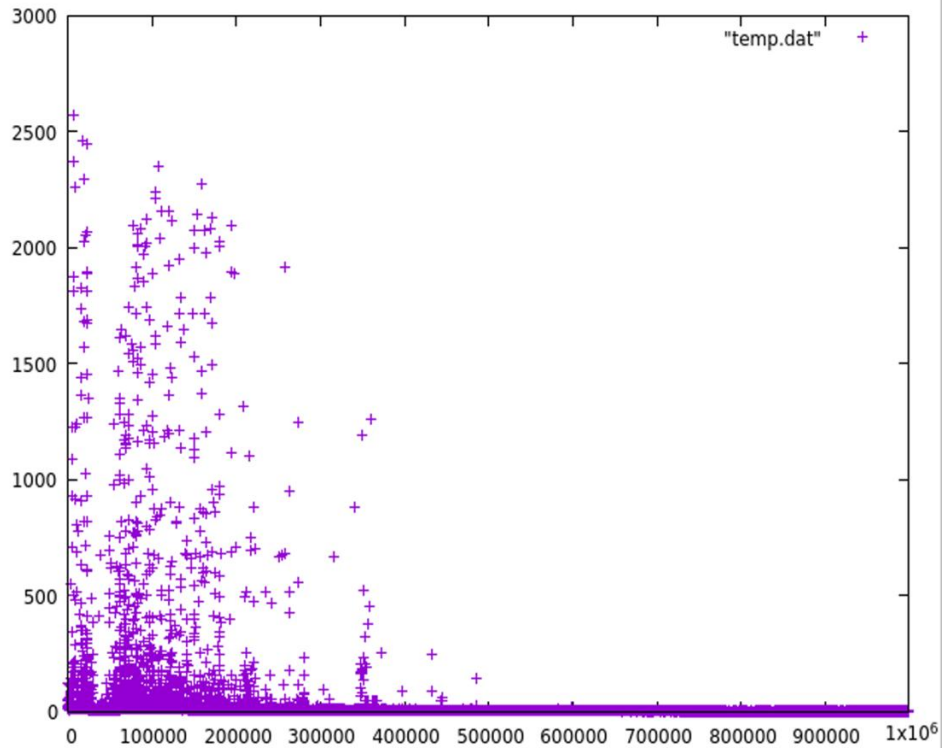


Fig. 14. The temperature for 100 particles with fields 110

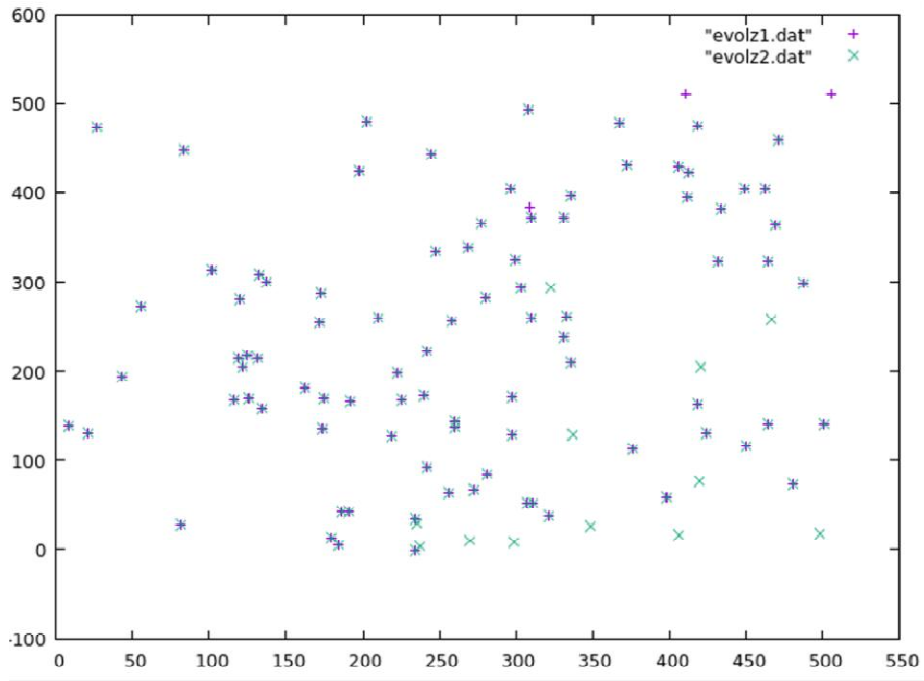


Fig. 15. Final configuration for 100 particles with fields 101; Red “+” denotes e-particles and green “x” denotes p-particles; Nearly all paired up; Some small clusters. Temperature at zero after 500,000 iterations; Shown in Fig. 16

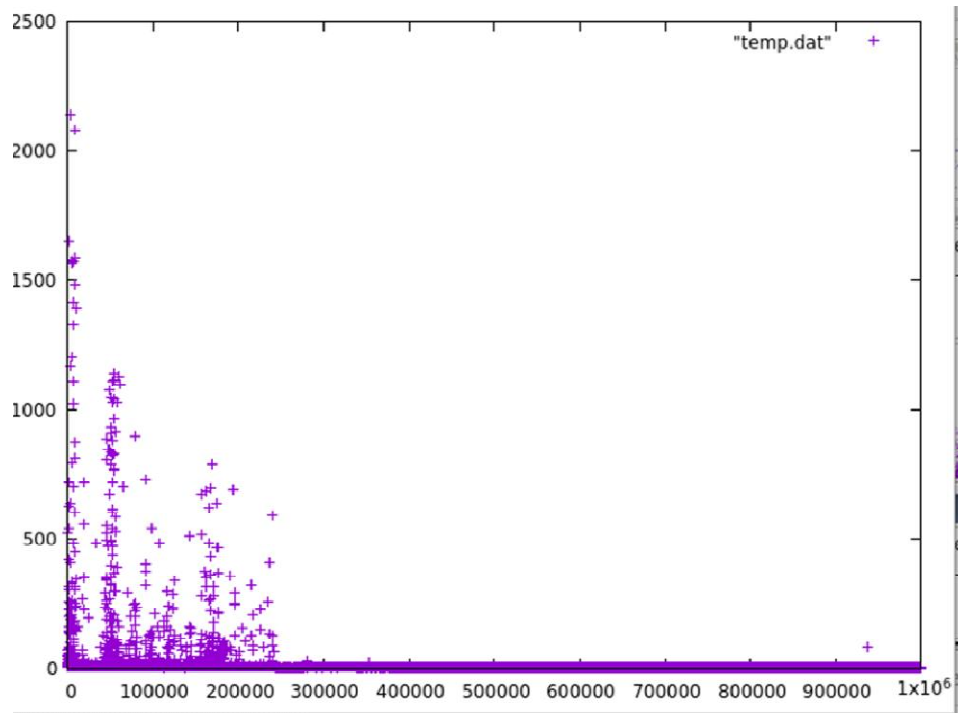


Fig. 16. The temperature 100 particles with fields 101

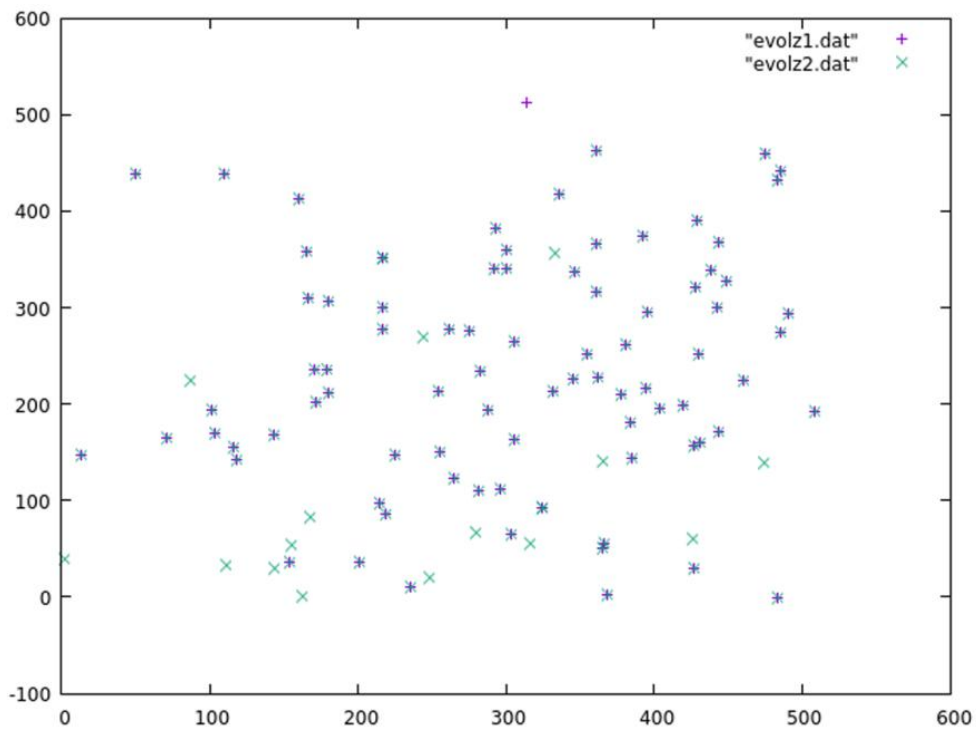


Fig. 17. Final configuration 100 particles with fields 011; Red “+” denotes e-particles and green “x” denotes p-particles; Mostly paired up; Temperature zero after about 700,000 iterations as displayed in Fig. 18

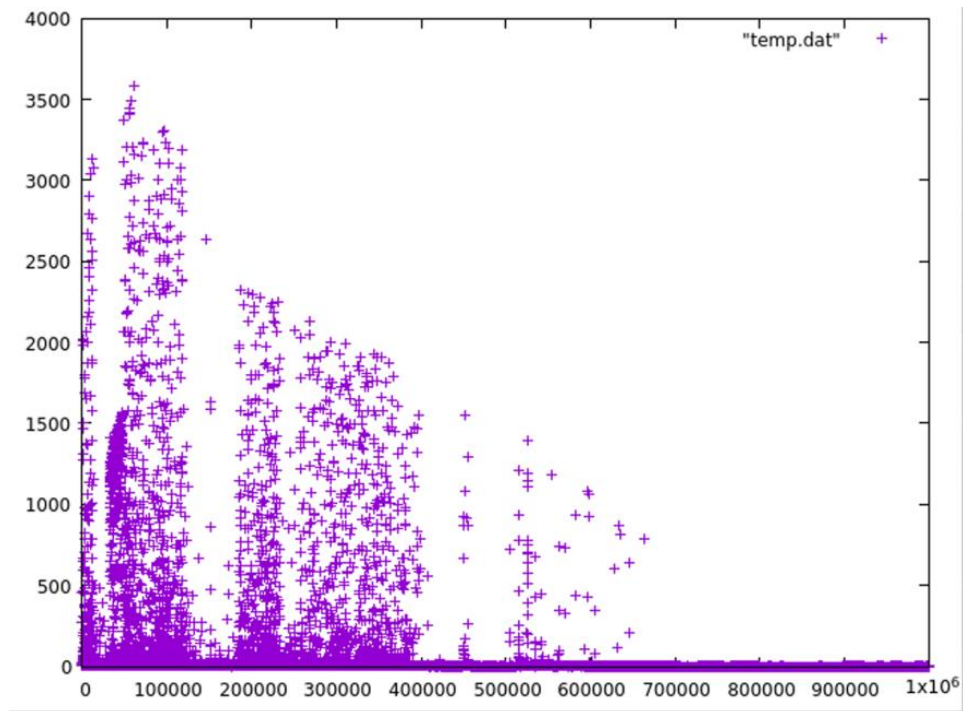


Fig. 18. The temperature for 100 particles with fields 011

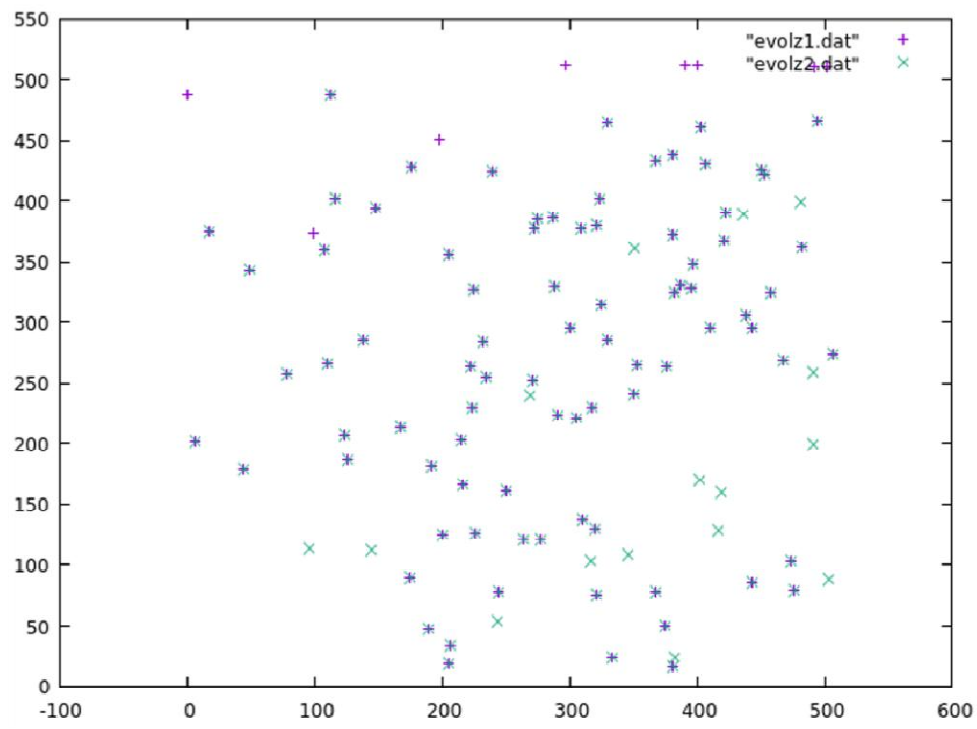


Fig. 19. Final configuration for 100 particles with fields 111; Red "+" denotes e-particles and green "x" denotes p-particles; Mostly paired up, but Fig. 20 shows there was still some movement after 1m iterations.

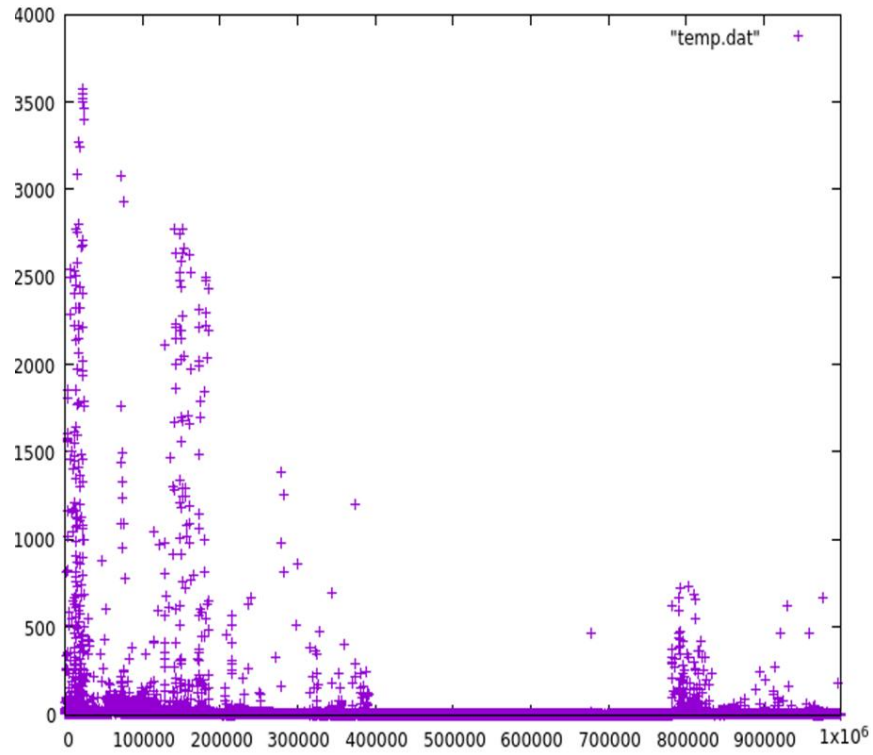


Fig. 20. The temperature for 100 particles with fields 111

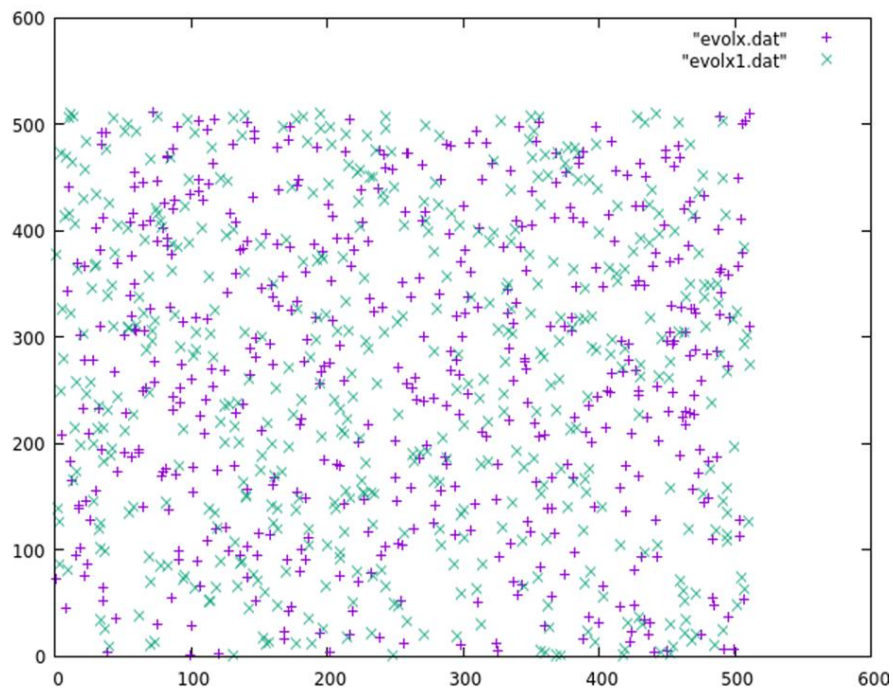


Fig. 21. Initial configuration for 500 particles; Red "+" denotes e-particles and green "x" denotes p-particles

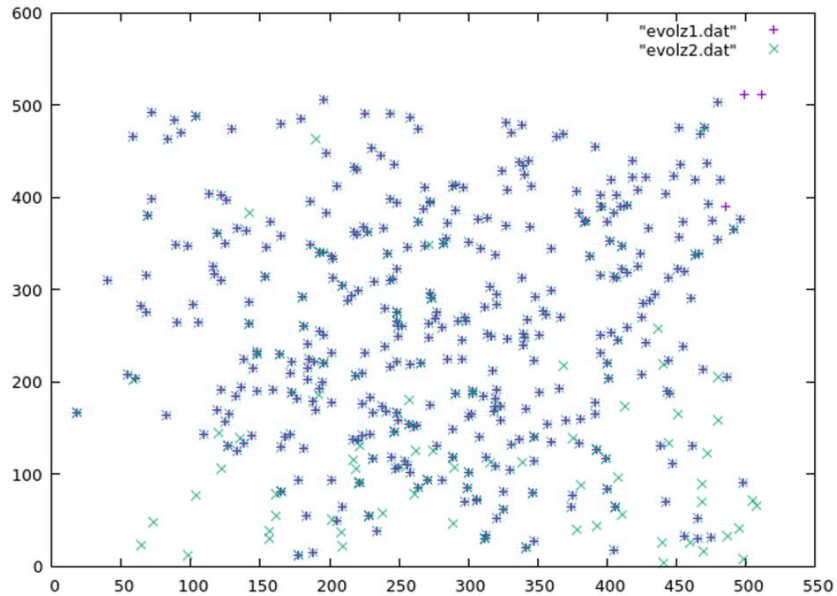


Fig. 22. Final configuration for 500 particles with fields 111; Red “+” denotes e-particles and green “x” denotes p-particles; Almost all paired up with some small clusters. Temperature Fig. 23 zero after 300,000 iterations

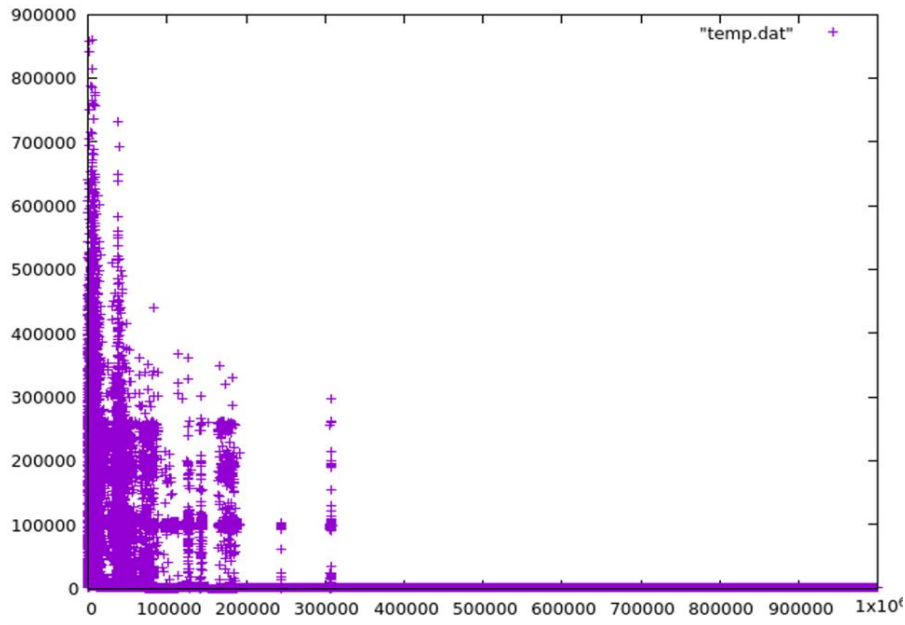


Fig. 23. The temperature for 500 particles with fields 111

4. DISCUSSION, CONCLUSION AND FUTURE WORK

Our objectives of this work were to explore self-organization using systems of few particles and simple dynamics and to investigate the effects of

an external E-field. We have presented the results of several experiments here and in other applications to demonstrate this approach [10]. There were two kinds of particles that interacted through the inverse square law under the influence of an external E-field. Starting from a

disordered state the system usually ended in an ordered state. We noticed that as the number of particles increased the likelihood of the system getting caught in a local minimum increased. This is a common circumstance in gradient descent methods.

One thing is clear from the results, in the presence of an E-field the pairing up of the particles and the system reaching a state of equilibrium was hastened. As stated earlier for the 100 particle case with no E-field the number of iterations for equilibrium was 20,000,000-30,000,000 iterations. Here, the equilibrium was achieved with just 1,000,000 or fewer iterations. It is not entirely clear why this is true. It could be partly due to the increased movement of the particles caused by the presence of an E-field. A second thing observed was that there were no sizeable clusters formed. The clusters that were formed contained 2-4 particles. This result may change for larger E-fields. This investigation is saved for future work.

This paper only reports results for a small number of configurations and a small number of parameters. The forces can be adjusted as to which particles interact with each other. Presented here is a program or simulation to describe the migration of particles under various scenarios. The program can give results for a fairly wide range of conditions. The forces can be adjusted to be attractive or repulsive and could be changed further by changing the program. Future work will expand this range and look for interesting scenarios to simulate.

COMPETING INTERESTS

Author has declared that no competing interests exist.

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