Gaslab - Gas in a Box

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1. Abstract

For this project, we decided to compare the model Chaos in a Box to the model Gas in a Box. Used in the fields of chemistry and physics, the Gas in a Box model is a simple system consisting of gas particles enclosed in a box; the path of a single particle is then visualized by a gray colored trace of the particle's most recent positions. In the Gas in a Box model, the basic idea is that gas particles are presumed to move and collide with either other particles or with any other objects such as walls. Like all of the GasLab models, the Gas in a Box model uses the same basic principles to simulate the behavior of gasses although each GasLab model integrates different features to highlight different aspects of gas behavior. Lastly the Gas in a Box model is part of the Connected Mathematics "Making Sense of Complex Phenomena" Modeling project. We decided to compare the Gas in a Box model to the Chaos in a Box model because they both model the movement of particles in a closed box

2. Introduction

In the Chaos in a Box model, the collisions alter the trajectory of the balls and while the system primarily exhibits chaotic behavior, the system can show periodic behavior where the ball bounces around in a repeating pattern when the initial conditions are appropriate. We have used this model to explore chaotic and periodic behavior in simple systems as well as how small changes in initial conditions are sufficient to create chaotic behavior. We ran multiple experiments starting from a really simple system with just one ball and no obstacles to one that involved multiple balls and multiple obstacles. We observed chaotic and periodic behavior both with and without obstacles. When there are no obstacles the collision angles are quite predictable even though the path traversed by the ball is not. However, in the presence of obstacles, especially when balls collide with obstacles, the path traversed by the ball can become highly unpredictable. As the size of the obstacle increases, the chances of collision increases making the system significantly more chaotic. Under appropriate initial conditions the system demonstrates periodic behavior. However, when those conditions change even slightly the effect becomes very chaotic. In the Gas in a Box model the particles are modeled as hard balls with no internal energy other than the internal energy that arises when the particle is in motion. In addition, like the Chaos in a Box model, the collisions between particles are elastic. Lastly, the particles are colored according to speed - blue for slow (speed less than 5), green for medium (above 5 and below 15), and red for high speeds (above 15)

3. Model Description

Our group decided to compare the Chaos in a Box model to the Gaslab model which was one of the models that was suggested by Netlogo and in particular, our group chose to write a review on the Gas in a Box model, which is one of several Gaslab models. The objective of the Gas in a

Box model is to simulate the behavior of gas particles in a closed box, or a container with a fixed volume. In the Gas in a Box model, gas particles are assumed to move and collide either with other particles or with any other objects such as walls. In addition, in the Gas in a Box model, the particles are represented as hard balls without any external energy other than the energy that is accumulated when the particles are in motion. Lastly, in the Free Gas model, collisions are elastic and particles are color coded according to their speed, with blue, green, and red representing slow, medium and red speeds respectively. In general, the overall notion behind the Gas in a Box model and all of the GasLab models is that gas particles are assumed to have two elementary actions: they move and they collide — either with other particles or with any other objects such as walls. The basic principle behind the Free Gas model and all of the GasLab models is the following procedure: A particle moves in a straight line while maintaining its speed unless it collides with another particle or bounces off the wall. Next two particles collide if they happen to be on the same patch. Next, a random axis is chosen, as if they are two balls that hit each other and this axis is the line connecting their centers. Next, the particles exchange momentum and energy along the created axis as per the laws of momentum and energy conservation. Lastly, each particle is assigned a new speed, heading and energy and if a particle finds itself on or very close to a wall of the container, it "bounces" — that is, reflects its direction and keeps its same speed

In the model, the important components are separated into three categories, initial and other settings, monitors, and plots. In the initial settings, the main components are NUMBER-OF-PARTICLES which gives the number of gas particles, INIT-PARTICLE-SPEED which determines the initial speed of each particle, PARTICLE-MASS which determines the mass of each particle, BOX-SIZE which displays the size of the box as a percentage of the world-width, the SETUP button which sets the initial conditions, and the GO button which runs the simulation. In other settings, the main components are TRACE? Which traces the path of one of the particles and COLLIDE? which turns collisions between particles on and off. In the monitors, the main components are FAST, MEDIUM, and SLOW which show the number of particles with different speeds: fast (red), medium (green), and slow (blue), AVERAGE SPEED which shows the average speed of the particles, and AVERAGE ENERGY which displays the average kinetic energy of the particles. Lastly in plots, the main components are SPEED COUNTS which plots the number of particles in each range of speed (fast, medium or slow), SPEED HISTOGRAM which shows the speed distribution of all the particles with the gray and black lines representing the average value and the initial average respectively. Lastly, ENERGY HISTOGRAM shows the distribution of energies of all the particles, calculated as (m*v^2)/2. In this monitor, the gray line is the average value, and the black line is the initial average. Moreover, since the particles all have the same speed and different, random directions, the speed and energy histogram plots only show one column each, however the plots will eventually change as the particle collisions become more frequent, energy between particles is exchanged and head off in directions, and therefore particle speeds are dispersed and change.

Compared to the Chaos in a Box model, which simply models the path of a ball as it moves around a box, the Gas in a Box model takes the Chaos in Box model one step further by having the ability to simulate the behavior of gasses in an closed environment in order to highlight different aspects of gas behavior and therefore, the Free Gas model can simply be thought of as an extension of the Chaos in a Box model. In addition, the Gas in a Box model is more complex and more informative than the Chaos in a Box model. For example, compared to the Chaos in a Box model where the user was only able to see the path of the ball as it moved around the box, in the Gas in a Box model, the user is able to see histograms of the particles' speed and energy as well as the percentage of the particles that are moving slow, medium, and fast in real time, both of which make the model more informative to the user. Moreover, some of the assumptions that are assumed to be true in the Gas in a Box model aren't necessarily the case in the Chaos in a Box model. For instance, the Gas in a Box model model assumes that there are no external constraints such as gravity or containers, and while this is to a certain degree true the Chaos in a Box model since gravity was also an nonexistent factor, the ball was relegated to being placed inside of a rectangular box and therefore, the ball was subject to external factors such as the walls of the box and any obstacles that happened to be placed in the box as well .

4. Simulation Results

To determine the similarities and differences between the two models we ran a number of trials with varying parameters. As done in our previous report, we investigated the chaos in the box model by running the simulation with different numbers of obstacles, varying their size, initializing different setup conditions, and using more than one ball. For run 1 we ran the simulation with no obstacles present using the random setup. Similar to our previous report, we observed that the movement of the object was periodic (**Figure 1**). However, when initializing an obstacle in the simulation this periodic behavior ceases to occur. In run 2, we initialized an obstacle of size 1 at coordinates (5,5) (**Figure 2**). Here, we noted that the ball's trajectory is periodic until it hits the obstacle and becomes chaotic. After a few seconds the trajectory again becomes periodic until hitting the obstacle once more. This behavior is again observed in run 3, where we initialized an obstacle of size 2 at coordinates (5,5) (**Figure 3**). The ball exhibits periodic behavior when the obstacle does not perturb it from its path. For run 4 we initialized an obstacle of size 3 at coordinates (5,5) (**Figure 4**). Here, we observed that the increase in obstacle size resulted in the ball being more likely to come into contact with the obstacle and therefore exhibit more chaotic behavior.

To gain further insight into the Chaos in a box model we initialized different setup conditions for the simulation. For run 5 we used the periodic-x setup option. This setting initializes an obstacle of size 3 at coordinates (0,0) (**Figure 5**). After running this simulation we noted that despite having an obstacle present in the box the ball still exhibited a periodic trajectory. However, moving the obstacle to the right just 0.1 resulted in chaotic behavior (**Figure 6**). Similarly, increasing the size of the obstacle to 4 also resulted in the ball exhibiting chaotic behavior (**Figure 7**). For run 6 we used the periodic-quilt setup, which initializes an obstacle of size 1 at coordinates (0,8) (**Figure 8**). Similar to run 5, despite there being an obstacle present in the box the ball's trajectory was periodic. Making a miniscule adjustment in the coordinates of the obstacle by moving it to the right by 0.1 (**Figure 9**), as well as changing the size, resulted in chaotic behavior for the ball's trajectory (**Figure 10**).

Next, we ran the chaos in the box model with two balls using the periodic setup option. The 'two-balls?' option sets the initial positions and directions of the two balls close to each other but not exact. This resulted in one of the balls exhibiting chaotic behavior while the other exhibited periodic behavior (**Figure 11**). One important thing to note is that although the two balls behaviors diverged upon hitting the obstacle, they remained similar when coming into contact with the walls of the box (**Figure 12**).

A number of runs were also performed on the gas in a box model. For run 1 we initialized the number of particles to 1 with an initial particle speed of 10, particle mass of 1, and a box size of 95% (**Figure 13**). We observed that the behavior of the trajectory of the particle was periodic, similar to the chaos in a box model when no obstacles are present. In addition, when only one particle is present, its speed and energy are constant at around 10 and 50, respectively. For run 2 we initialized the number of the particles to 6 and turned on the collide option (**Figure 14**). In addition, the initial particle speed was set to 10, particle mass to 11, and box size to 95%. We observed that the particle's trajectory exhibits periodic behavior until it collides with another particle. In addition, we noted that the speed of the particles was mainly medium (50%), followed by slow (33%) and fast (17%). We also observed that the average speed of the particles fluctuated between 8.6 and 9.4 with an average energy of 50. For run 3 we initialized the number of particles to 501 with the collide option on (**Figure 15**). The initial particle speed was set to 10, particle mass to 11, and box size to 95%. Here, we observed that increasing the number of particles to 501 resulted in the particle no longer exhibiting a periodic trajectory throughout any point in the trajectory. We also noted that the speed of the particles was distributed as 68% medium, 21% slow, and 11% fast. In addition, the simulation results showed that the average speed ranged from 8.8 to 9.6. With an average energy of 550.

Next, we ran a number of trials to identify how the initial particle speed affects the model. For run 4 we set the number of particles to 104 and set the collide option on (**Figure 16**). The initial particle speed was set to 1, the particle mass was set to 11, and the box size was set to 95%. We observed that all the particles stayed at a slow speed for the entirety of the simulation. In addition, we noted that the average speed stayed at approximately .89 with an average energy of 5.5. For run 5 we kept all parameters the same as in run 4 except for initial particle speed, which was increased to 10 (**Figure 17**). We observed there was a mix of particles of different speeds present throughout the entire simulation. The medium speed particles were more persistent at about 70%, followed by the slow and fast speeds at 22 and 8 % respectively. Additionally, We noted that the average speed was approximately 8.9% with an average energy of 550. For run 6 we kept all parameters the same as the two previous runs and changed the initial particle speed to 20 (**Figure 18**). As in run 5, we observed a mix of particles of different speeds present throughout the entire simulation, however, this run was most populated by the fast speed particles 57% and followed by the medium 38% and slow speed 5% particles.

5. Conclusions and Future Work

For our project we compared two models, “Chaos in a Box” and “Gas in a Box”. When running the Chaos in a Box model we observed that the ball exhibited a periodic trajectory when no obstacles were present and similar behavior was seen in the “Gas in a Box” model when only one particle was initialized in the simulation. As a result, we came to the conclusion that an object that displays chaotic behavior will converge to some periodic trajectory as long as there are no obstacles that will perturb its path. This is further supported by the subsequent runs that included obstacles in the simulations. In the “Chaos in a Box” model we noted that when an obstacle is initialized the ball no longer converges to some periodic trajectory. Similarly, when more than 1 particle is present in the “Gas in a Box” model, the particle being traced ceases to exhibit a periodic trajectory. One interesting fact that we observed was that while there were certain conditions where including an obstacle resulted in a periodic trajectory for the “Chaos in a Box” model, there were no conditions where including more than one particle resulted in a periodic trajectory for the “Gas in a Box” model. This is most likely due to the fact that in “Chaos in a Box” the obstacle is stationary while in “Gas in the Box” the particles move. As a result, we conclude that initial conditions must be constant in order for an object to converge to a periodic trajectory.

When running the gas in a box model we noted that when particles of different speeds collided their respective speeds changed depending on the speed of the other particle. For example, if a fast particle collided with a slow particle both would end up as medium speed particles. We also observed that when more high speed particles were present the energy present was higher. In addition, increasing the particle mass also increased the amount of energy present. This is due to the fact that total energy = (½)*n*mass*v^2 where n and v represent the number of gas particles and initial speed of the gas particles respectively.

total momentum before = total momentum after

$$m_A v_A + m_B v_B = m_A v'_A + m_B v'_B$$

total kinetic energy before = total kinetic energy after

$$\frac{1}{2} m_A v_A^2 + \frac{1}{2} m_B v_B^2 = \frac{1}{2} m_A v_A'^2 + \frac{1}{2} m_B v_B'^2$$

Therefore, this model follows the law of conservation of energy which states that energy cannot be destroyed or created, only converted. This is shown in the simulations where the individual energy levels of particles increase or decrease upon collision with another particle but the overall energy of the system remains constant.

Both models have the capability of simulating chaotic motion within an isolated environment. However, to gain insight into more realistic systems they must be extended. The “Chaos in a Box” model could be modified to include different sizes of balls as well as include the option to change the speed of each initialized ball, similar to what “Gas in a Box” does. The “Gas in a box” model on the other hand, can be extended to include stationary obstacles in order to replicate conditions where a particle’s trajectory is periodic. Both these models are simulated on a 2-dimensional plane, however, they would be more applicable to realistic conditions if they were simulated on a 3-dimensional plane. In addition, they would better represent real world condition if rather than acting as perfectly elastic, the objects behaved imperfectly elastic.

6. References/figures

References

1. Head, B. and Wilensky, U. (2017). NetLogo Chaos in a Box model. http://ccl.northwestern.edu/netlogo/models/ChaosinaBox. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.
2. Wilensky, U. (1999). NetLogo. http://ccl.northwestern.edu/netlogo/. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.
3. Aguirre, Luis A., and Christophe Letellier2. "Modeling Nonlinear Dynamics and Chaos: A Review." *Mathematical Problems in Engineering*, vol. 2009, 2 June 2009, pp. 1-35. *https://scholar.google.com/*, doi:10.1155. Accessed 9 Feb. 2020.
4. Wilensky, U. (1997). NetLogo GasLab Gas in a Box model. http://ccl.northwestern.edu/netlogo/models/GasLabGasinaBox. Center for Connected Learning and Computer-Based Modeling, Northwestern University, Evanston, IL.
5. Math 168 Chaos in a box, Project 1.2020 Spring

Figures

Figure 1: No Obstacles in box

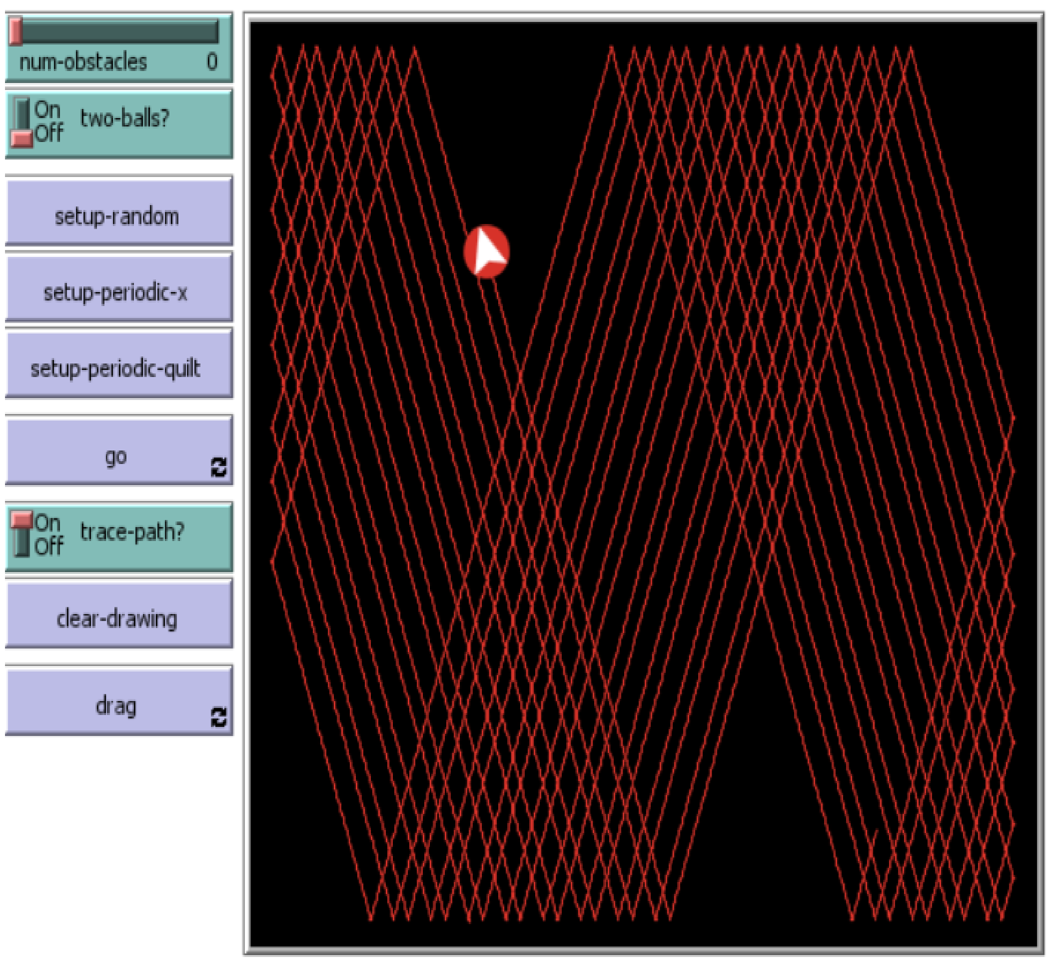

Figure 2: Obstacle of size 1 at (5,5)

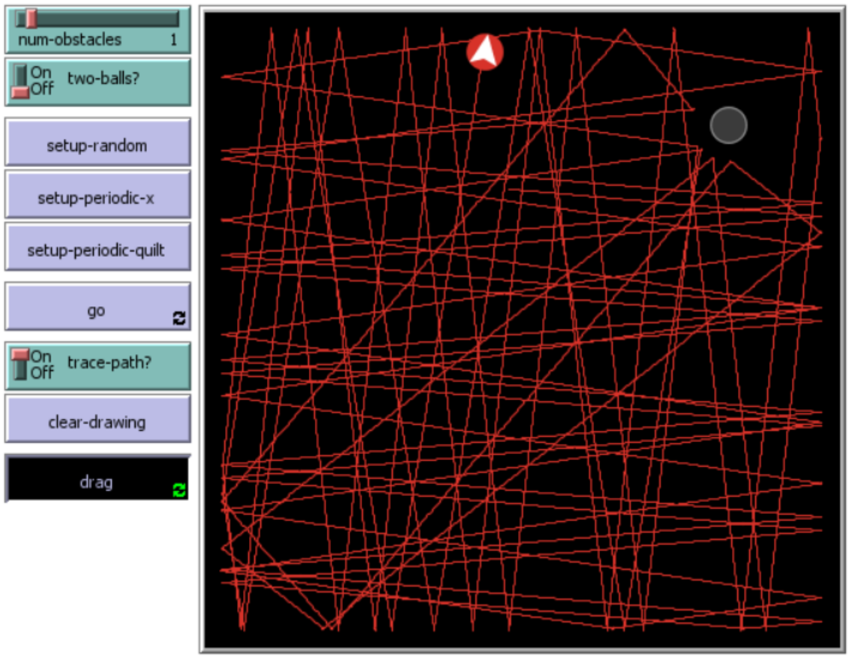

Figure 3: Obstacle of size 2 at (5,5)

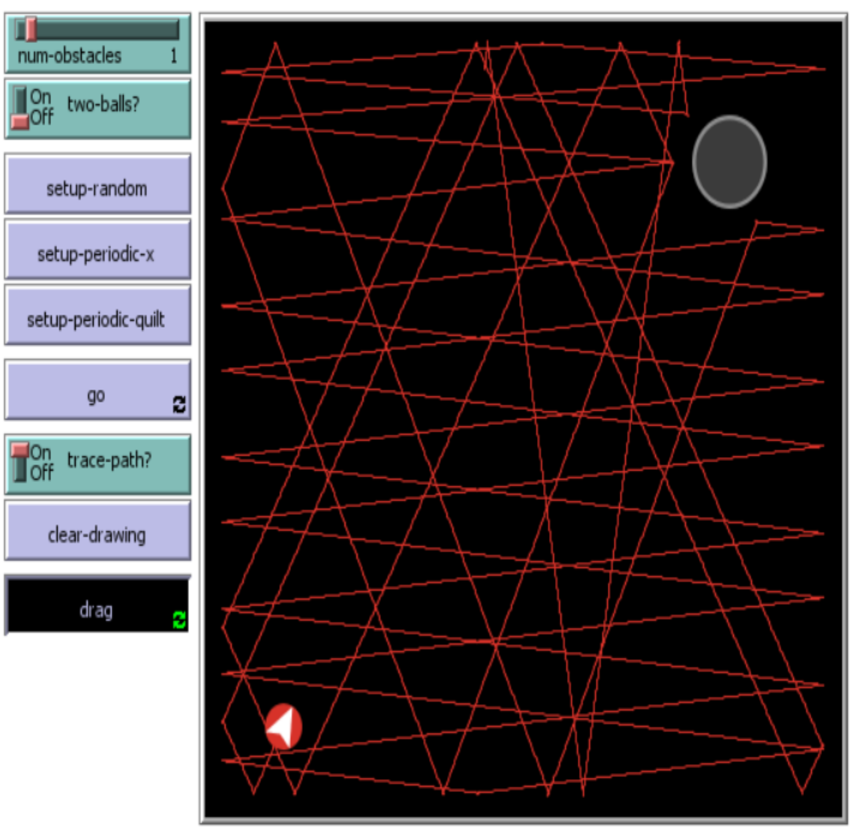

Figure 4: Obstacle of size 3 at (5,5)

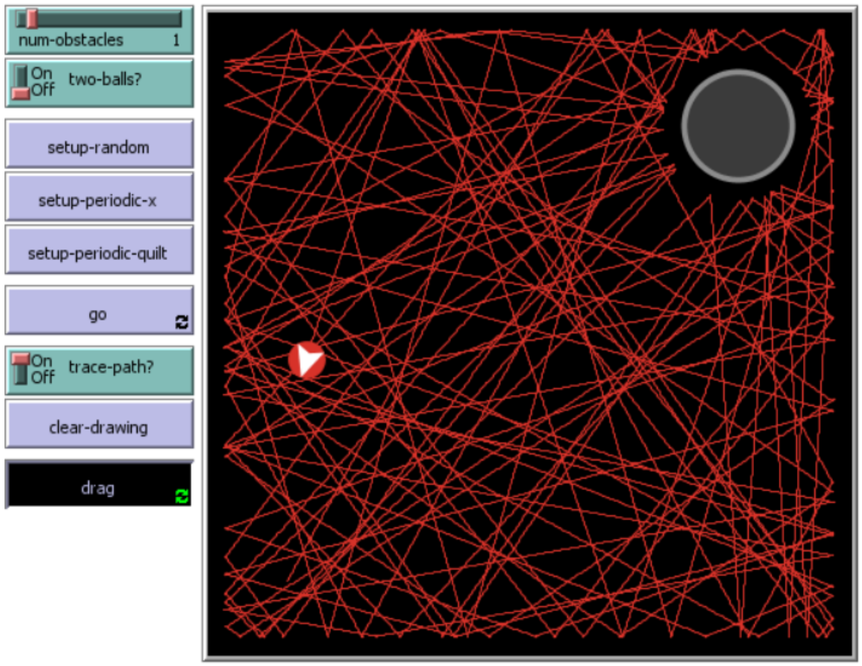

Figure 5: Setup periodic-x option with 1 ball

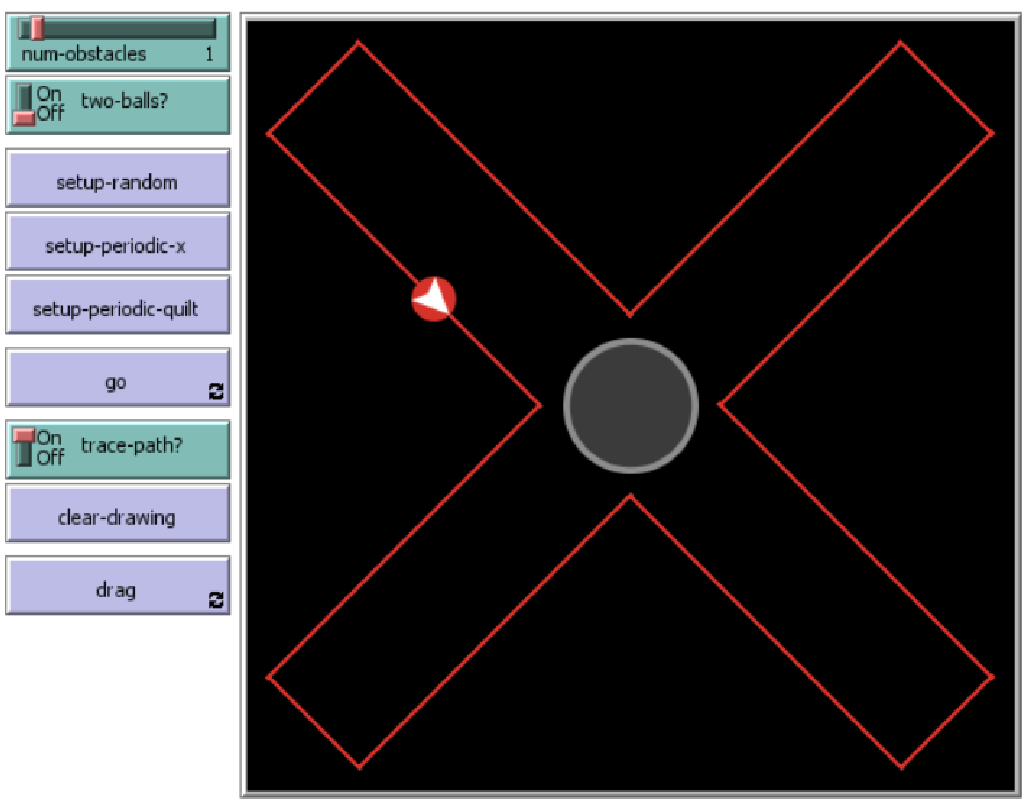

Figure 6: Set up periodic-x option with obstacle moved to the right 0.1

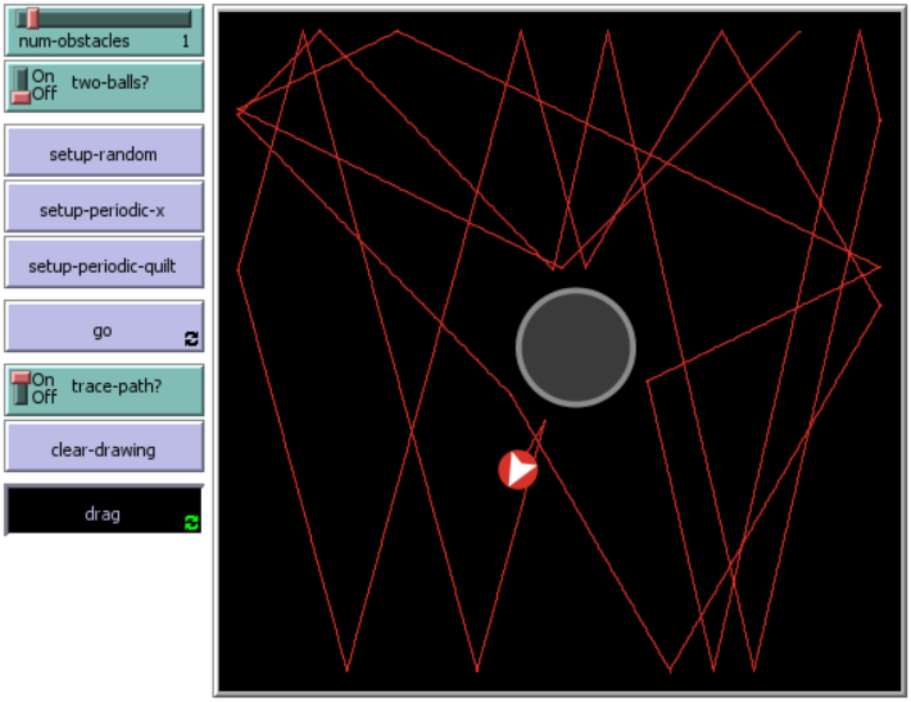

Figure 7: Setup periodic-x option with obstacle size 4

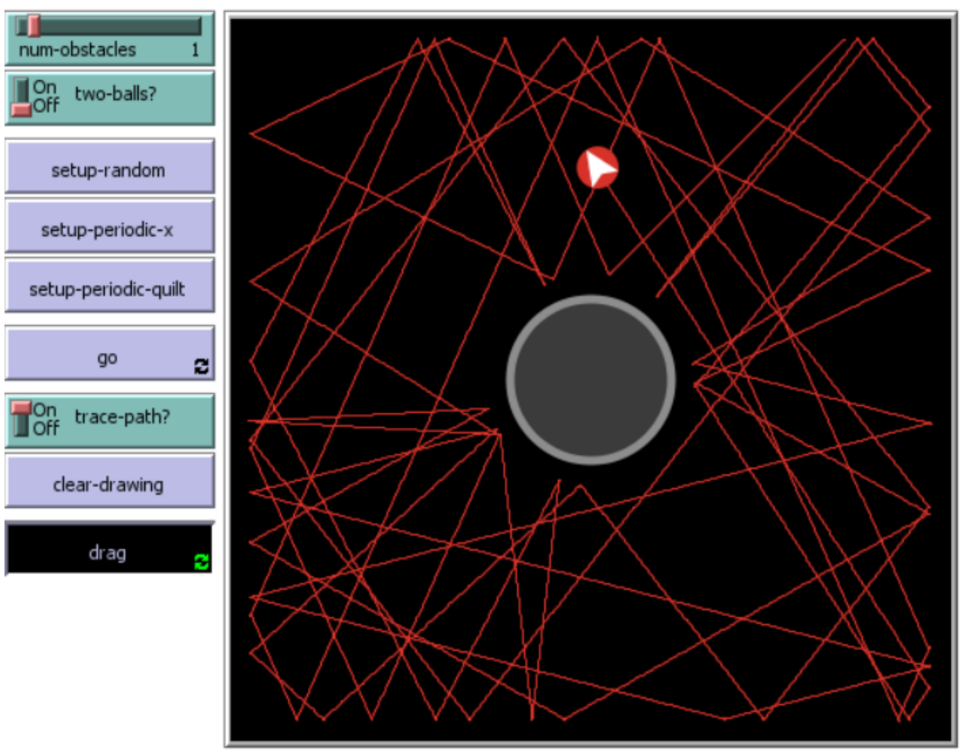

Figure 8 Setup periodic quilt option

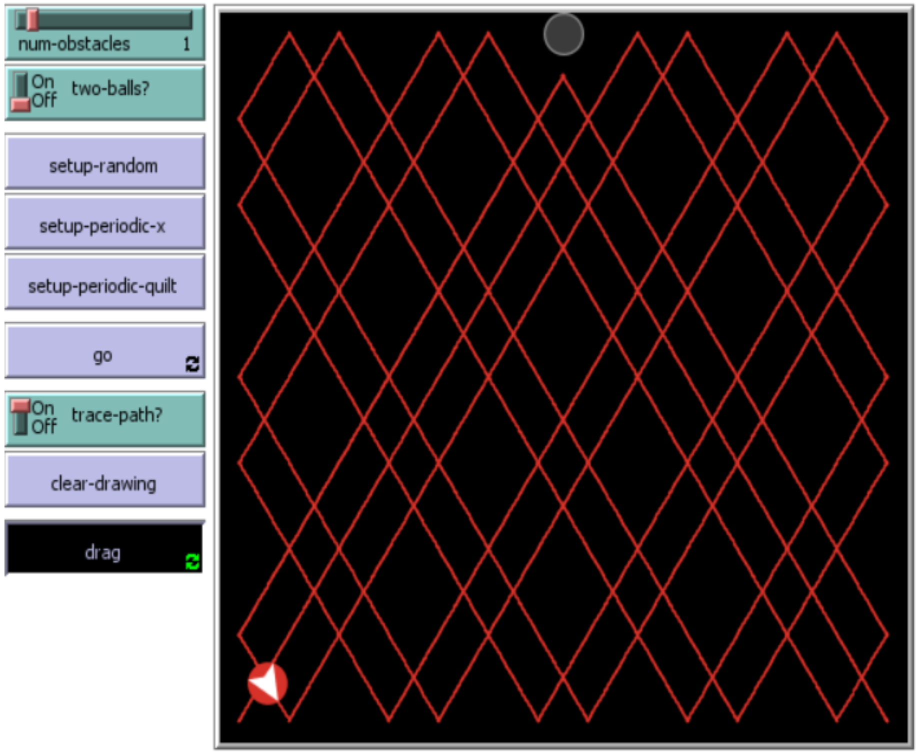

Figure 9: Set up periodic quilt option with obstacle moved to the right 0.1

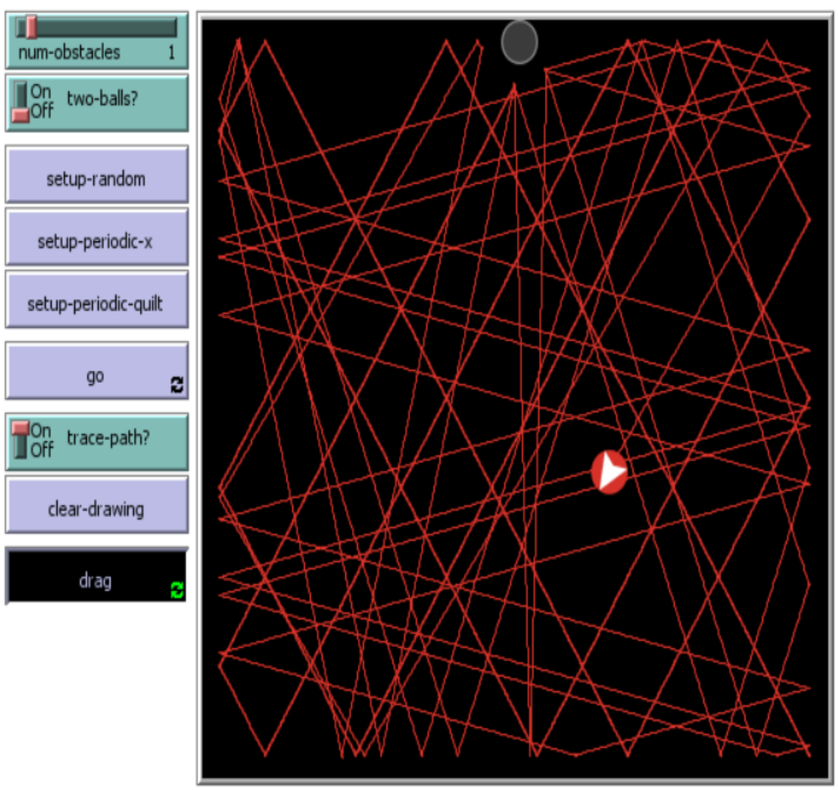

Figure 10 :Setup periodic quilt option with obstacle size 4

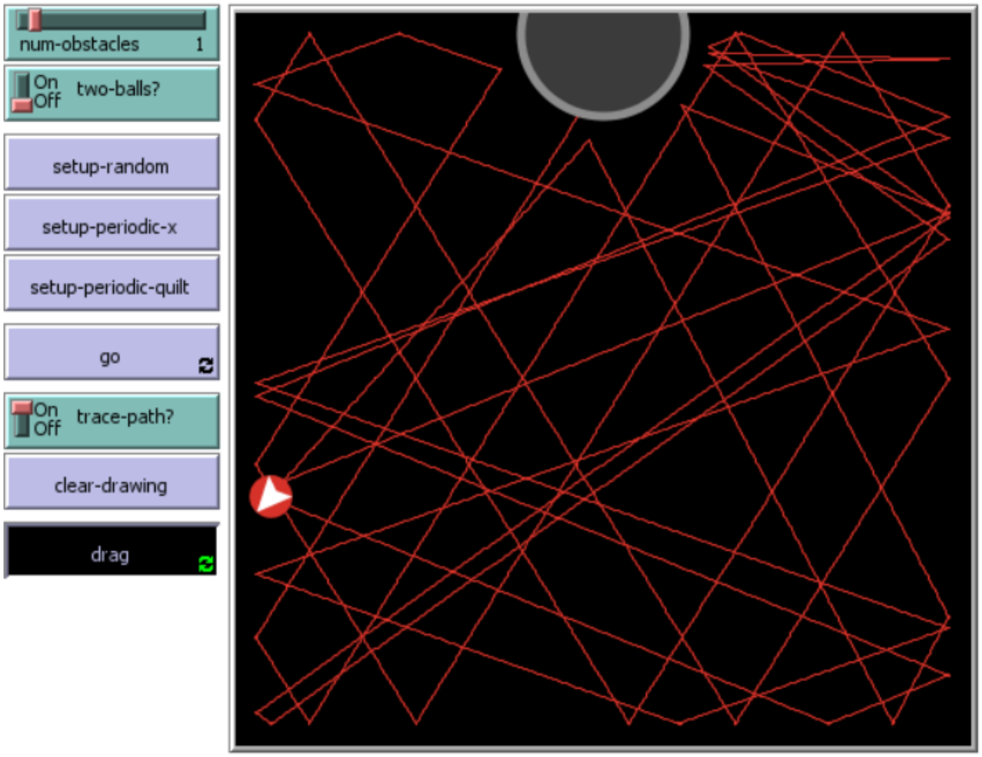

Figure 11: Setup periodic-x option with ‘two balls?’ option turned on

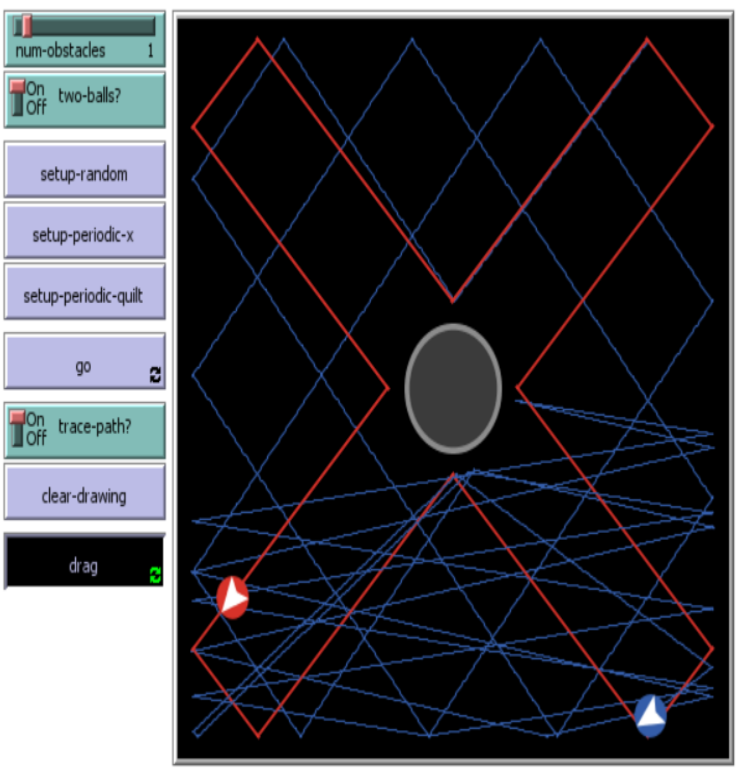

Figure 12: Setup random with ‘two-balls?’ option turned on

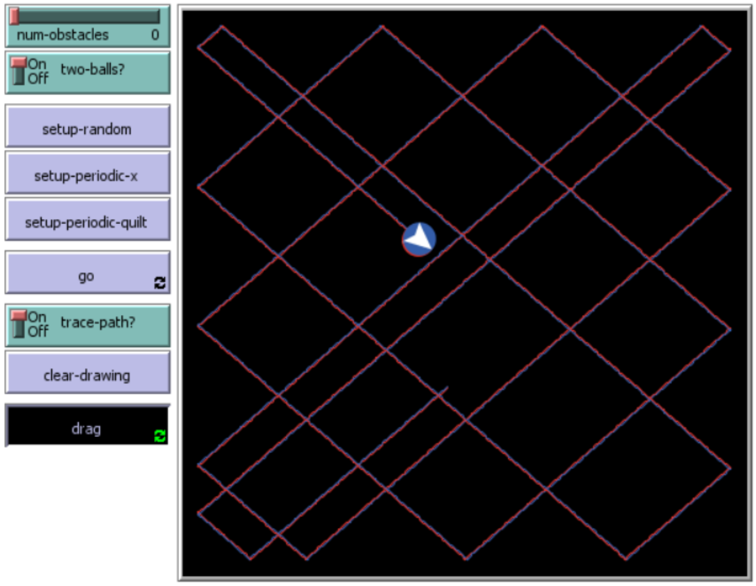

Figure 13:1 particle, initial speed 10, particle mass 1, and box size 95%

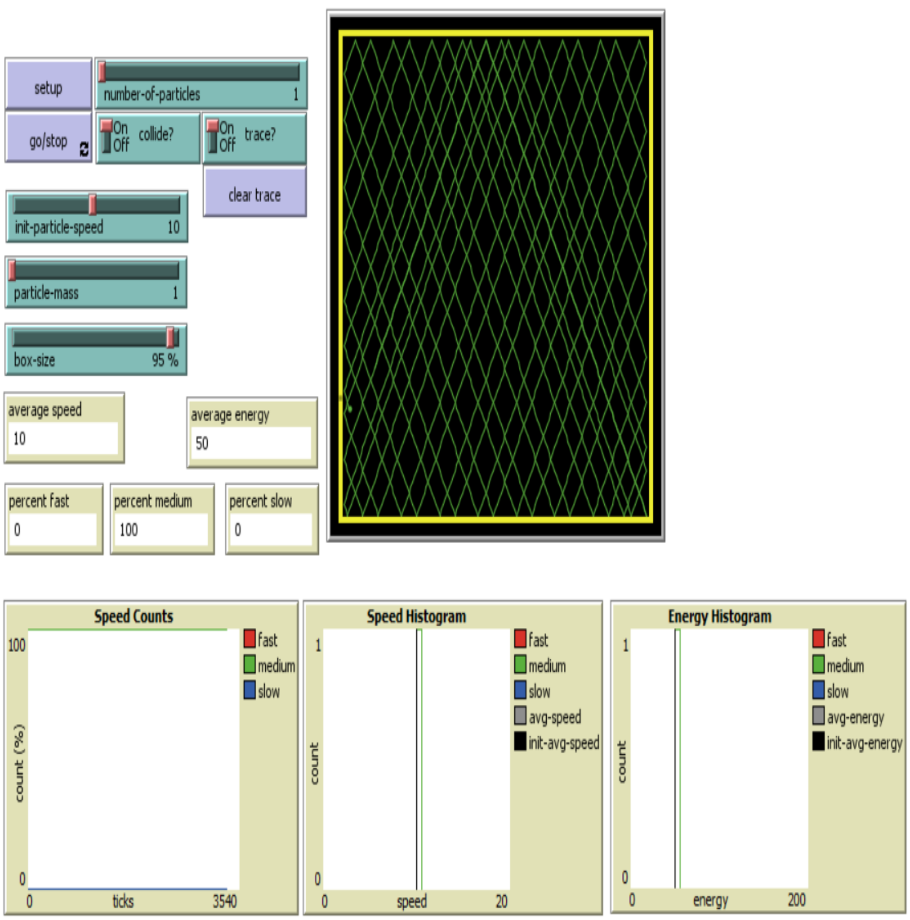

Figure 14: 6 particles, initial speed 10, particle mass 1, box size 95%

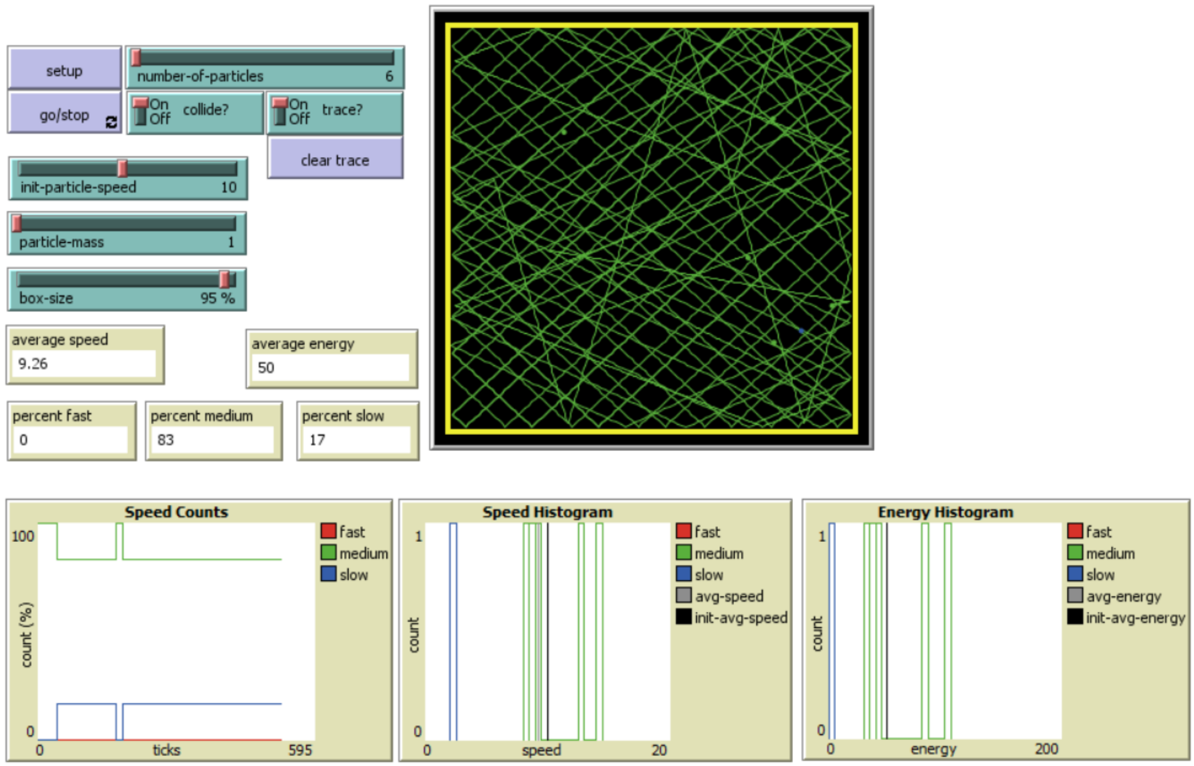

Figure 15: 501 particles, initial speed 10, particle mass 11, box size 95%

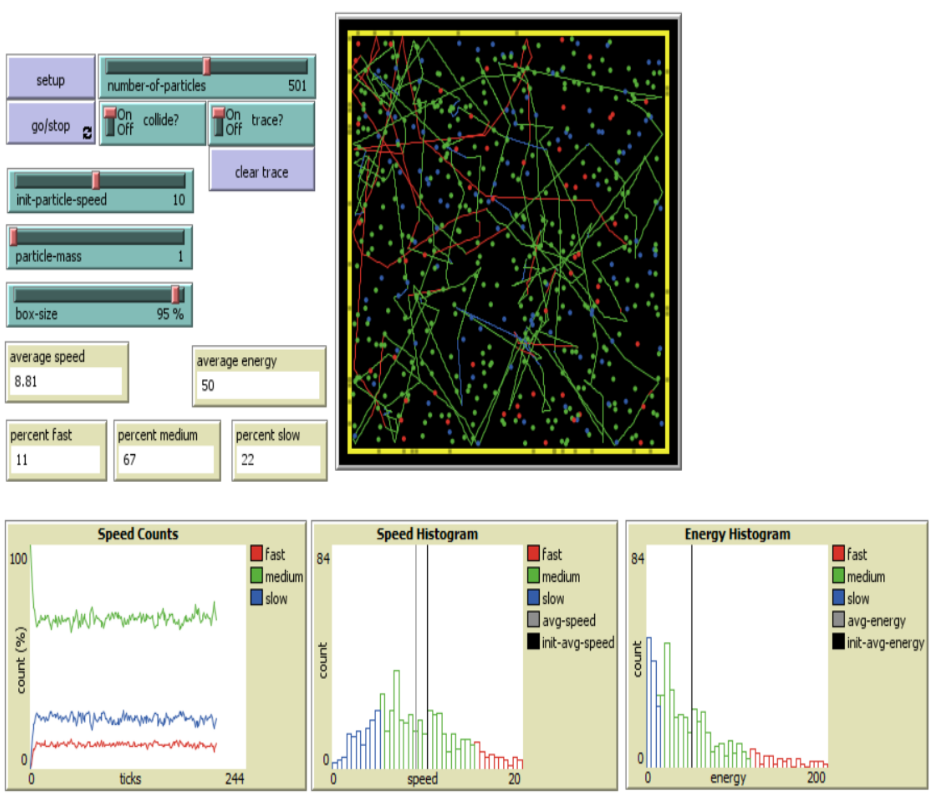

Figure 16: 104 particles, initial speed 1, particle mass 11, and box size 95%

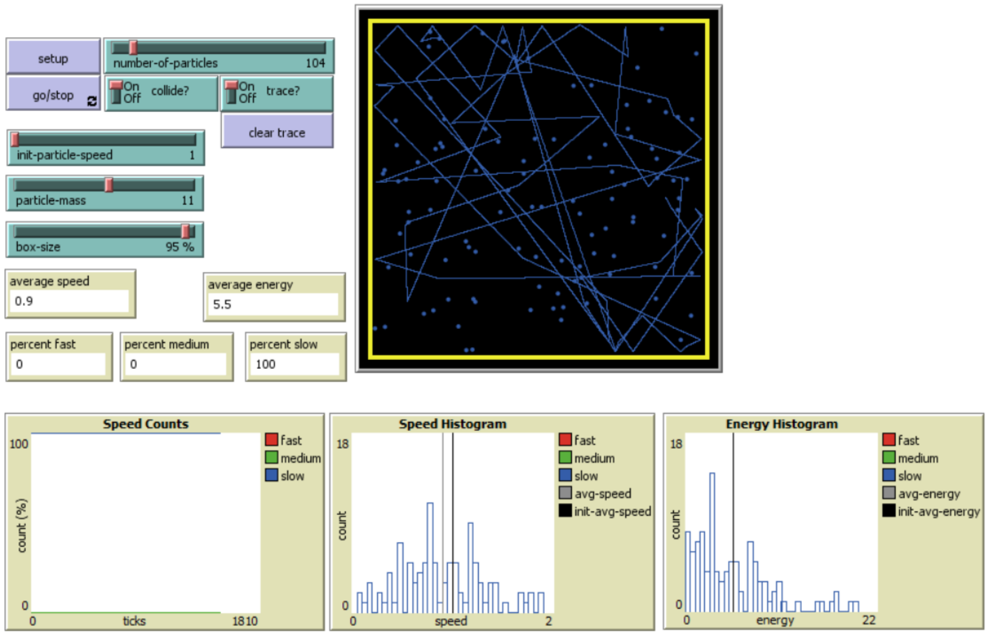

Figure 17: 104 particles, initial speed 10, particle mass 11, box size 95%

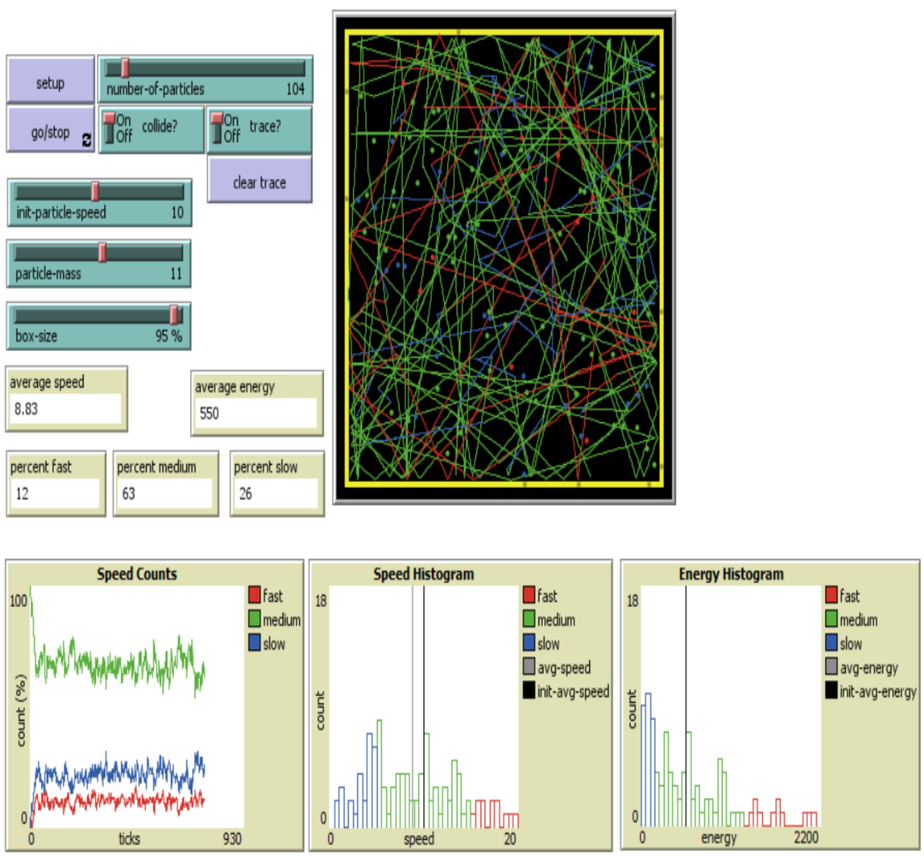

Figure 18: 104 particles, initial speed 20, particle mass 11, box size 95%