Università degli studi di Torino

Fisica dei sistemi complessi

Simulation of a Totally Asymmetric Simple Exclusion Process (TASEP) to model vehicular traffic.

Benedetta Mariani

November 8, 2018

Abstract

The aim of this work is to reproduce the dynamics of a Totally Asymmetric Simple Exclusion Process through an agent based simulation on NetLogo. A TASEP is a traffic model that can be analytically studied. It is based on a one-dimensional lattice, where the particles are injected and extracted with fixed rates, and move only rightward if the adjacent site is empty. Varying these rates, the system displays different phases of the stationary state. I will compare the results of my simulation with the theoretical expected results in the different realizations of the dynamics.

Contents

1 Introduction to the theoretical model

The model I will consider in this work was firstly proposed in 1968-1969 ([1, 2]) to describe the kinetics of protein synthesis on the polyribosome, a biological traffic problem. Then the model became paradigmatic for vehicular traffic as well thanks to its relevance. The simplest version of this class of models, that I will consider in details here, is the Totally Asymmetric Simple Exclusion Process (TASEP) ([3]). It is defined on a one-dimensional lattice, where particles can hop only rightward, from each node to the adjacent one, provided the latter is empty (for example a car on a one-lane road moves forward provided there is not a vehicle in front of it) at unit rate.
To study in detail this model it is necessary to label lattice nodes from left to right by $i = 1, ..., N$ and to introduce random variables of the occupation number type $n_i^t = 0, 1$, where $n_i^t = 1$ if node i is occupied by a particle at time t and $n_i^t = 0$ otherwise. I will use local densities, defined as the expectation values of the occupation number of site i at time t: $\rho_i^t = \langle n_i^t \rangle$. Here I will consider the case of open boundary conditions, with particles injected at the leftmost node (provided it is empty) with rate α, and extracted from the rightmost node (provided it is occupied) with rate β. An equivalent description may be obtained assuming that the system is in contact with two reservoirs of fixed densities α ahd $1 - \beta$, which respectively inject and extract particles.

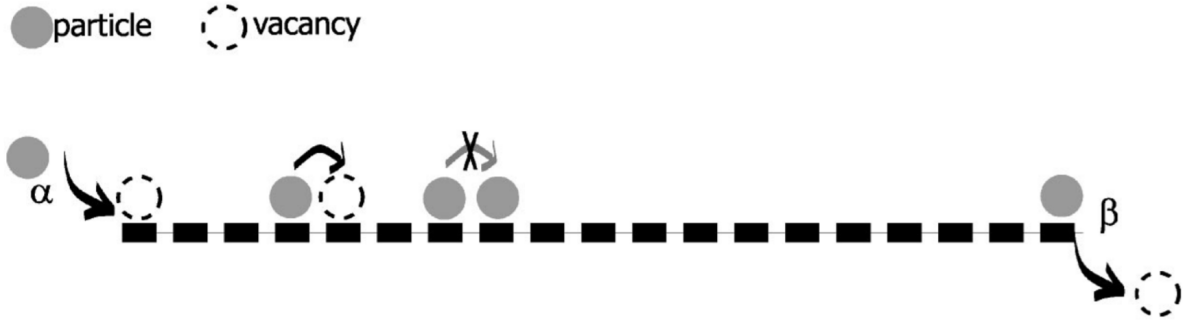

Figure 1

1.1 The stationary state

To study analitically the TASEP dynamics it is necessary to study the time evolution of expectation values. Starting with the local densities we obtain simple discrete continuity equations:

$$\dot{\rho}_i^t = J_{i-1}^t - J_i^t \qquad i = 1, ..., N$$

where J_i^t denotes the rightward current which exits from node i at time t. We have that

$$J_i^t = P(n_i^t = 1, n_{i+1}^t = 0) \qquad i = 1, ..., N-1,$$

with the boundary conditions

$$J_0^t = \alpha(1 - \rho_1^t) \qquad J_N^t = \beta \rho_N^t$$

Solving this model is non-trivial, although an exact solution for the stationary state exists. The simplest approximation one can resort to is mean-field, where one assumes that at each time t the joint probability distribution factors into single-node marginals. The local currents are so given by:

$$J_i^t = \rho_i^t(1-\rho_{i+1}^t) \qquad i = 1, ..., N-1.$$

and the continuity equations describing the time evolution of the local density become

$$\dot{\rho}_i^t = J_{i-1}^t - J_i^t = \rho_{i-1}^t(1-\rho_i^t) - \rho_i^t(1-\rho_{i+1}^t), \qquad i = 2, ..., N-1 \tag{1}$$

with the boundary conditions

$$\dot{\rho}_1^t = \alpha(1-\rho_1^t) - \rho_1^t(1-\rho_2^t) \qquad \dot{\rho}_N^t = \rho_{N-1}^t(1-\rho_N^t) - \beta\rho_N^t \tag{2}$$

As a first step, I will consider the stationary state of the model, where the local densities and currents become time-indipendent and will be denoted by ρ_i and J_i respectively. By continuity $\dot{\rho}_i = 0$ implies that the current is also uniform, that is

$$J_{i-1} = J_i \qquad i = 2, ..., N-1.$$

There will therefore be $J_i = J$ in the stationary state, and the density profile will be obtained by solving the equations

$$\rho_i(1-\rho_{i+1}) = J, \qquad i = 1, ..., N-1$$

with the boundary conditions

$$\rho_1 = 1 - \frac{J}{\alpha}, \qquad \rho_N = \frac{J}{\beta}$$

The above equations can be viewed as a set of N + 1 equations in the N + 1 unknown J and $\rho_1, ..., \rho_N$, to be solved at given values of the parameters α and β. Alternatively, it is possible to regard J and ρ_1 as the given parameters and solve for the density profile using the recursion

$$\rho_{i+1} = 1 - \frac{J}{\rho_i}, \qquad i = 1, ..., N \tag{3}$$

and eventually computing α and β from the boundary conditions.
In the large N limit it's legitimate to expect to find bulk solutions, characterized by a uniform density ρ, which must satisfy the condition

$$J = \rho(1-\rho) \leq \frac{1}{4}$$

This equation has solutions ρ_+ and ρ_-, which are the fixed points of the recursion Eq. (3) and satistfy $\rho_+ + \rho_- = 1$ and $\rho_+\rho_- = J$.
This recursion (Eq. (3)) can be solved exactly, but in order to understand the full

solution of the stationary state problem, it is convenient to start by considering the recursion relation and its fixed points for fixed value of J, and then returning to the original formulation of the stationary state problem, where we refer to α and β as input parameters. Considering the derivative of the recursion relation at the fixed points it is easy to check that ρ_- is an unstable fixed point of the recursion ($\frac{\partial \rho_{i+1}}{\partial \rho_i}|_{\rho_i=\rho_-} > 1$), while ρ_+ is stable ($\frac{\partial \rho_{i+1}}{\partial \rho_i}|_{\rho_i=\rho_+} < 1$).

1.1.1 The low-density phase

As a first analysis, let us consider as input parameter a ρ_1 sufficiently close to the unstable fixed point ρ_-: in this case the recursion will stay close to ρ_- for a sufficiently large number of steps, and then eventually reach some boundary value $\rho_N < \rho_+$. This means that in the large N limit the bulk density $\rho = \rho_- < \frac{1}{2}$ will extend to the left boundary. From the boundary conditions we obtain the injection rate $\alpha = \frac{J}{(1-\rho_-)} = \rho_- < \frac{1}{2}$ and the extraction rate $\beta = \frac{J}{\rho_N} > \frac{J}{\rho_+} = \rho_- = \alpha$. So, returning to the original formulation where I consider α and β as input parameters, it is possible to say that for $\alpha < \frac{1}{2}$ and $\alpha < \beta$ the stationary state of the system is a low-density (LD) phase (particles leave faster than they enter), with bulk density $\rho = \alpha < \frac{1}{2}$.

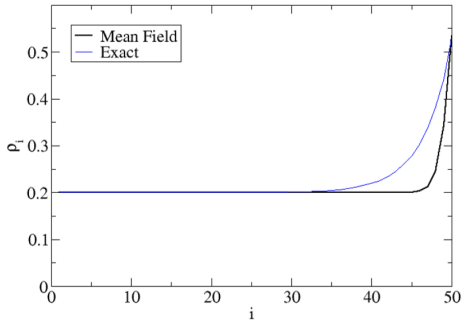

Figure 2: The density profile in the low-density phase (for N = 50, $\alpha = 0.2$, $\beta = 0.3$). It is evident the bulk plateau of the density at $\rho = \alpha$.

1.1.2 The high-density phase

Repeating this analysis for different values of ρ_1 and then returning to α and β as input parameters, it is possible to describe in terms of the parameters α and β different phases of the stationary state. In fact, for $\beta < \frac{1}{2}$ and $\beta < \alpha$ the stationary state of the system turns out to be a high-density (HD) phase (particles enter faster than they can leave), in which there is a bulk density $\rho = \rho_+ > \frac{1}{2}$ that extends to the right boundary. The bulk density is indeed equal to $\rho = 1 - \beta > \frac{1}{2}$.

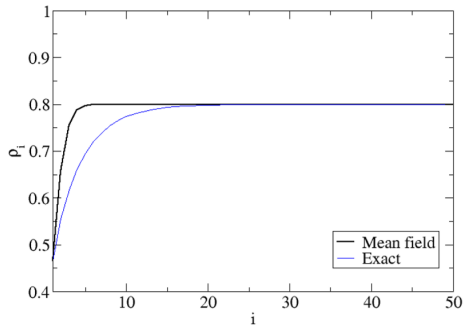

Figure 3: The density profile in the high density phase for N = 50, $\alpha = 0.3$ and $\beta = 0.2$. It is qualitatively symmetric to that of the low–density phase, and exhibits a bulk density equal to $\rho = 1 - \beta = 0.8$

1.1.3 The coexistence line

The two low and high-density phase are separated by the coexistence line $\alpha = \beta < \frac{1}{2}$. In this case a symmetric density profile is obtained, which, in the large N limit, exhibits two macroscopic bulk regions, separated by a domain wall: a low-density one, with density $\rho_- = \alpha$, extending to the left boundary, and a high-density one, with density $\rho_+ = 1 - \beta$, extending to the right. Notice that the bulk density is discontinous at the coexistence line, hence the corresponding transition is named discontinous.

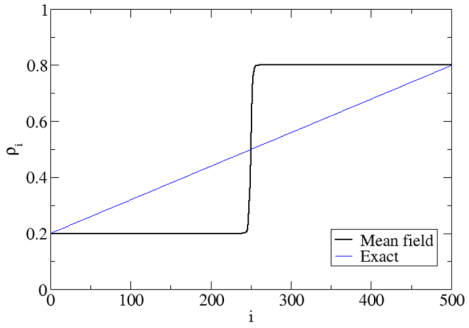

Figure 4: Density profile at the coexistence line, for N = 499, $\alpha = \beta = 0.2$. In the limit $N \to \infty$ the domain wall can be anywhere and an infinite number of solutions appears, whose average gives a linear prole in the exact solution

1.1.4 The maximal current phase

Finally, let us consider the case in which $\alpha > \frac{1}{2}$ and $\beta > \frac{1}{2}$. In this situation the stationary state is in a maximal current (MC) phase, where there is a central bulk region with density $\rho = \frac{1}{2}$ and a current $J = \frac{1}{4}$, which assumes its maximum possible value.

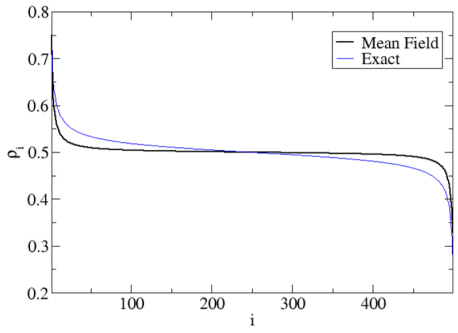

Figure 5: A typical density profile in the maximal current phase (for N = 499, $\alpha = \beta = 1$).

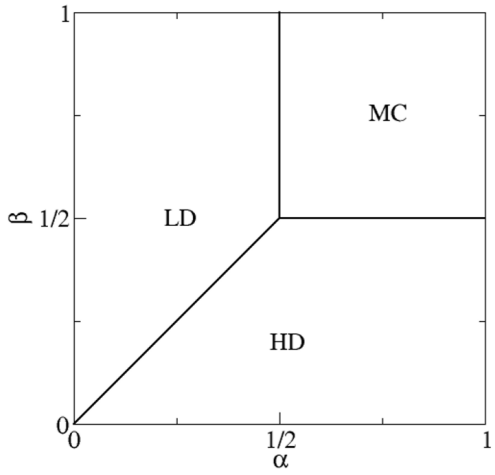

Figure 6: The stationary state phases as functions of α and β

1.2 Dynamics of the TASEP

I have discussed the stationary state. I can now turn my attention to the full dynamics, on which my simulation is based. Equation 3 is not valid anymore out of the stationary state, and the currents as well as the densities must be considered as time-dependent. So, the dynamics can be now analytically derived through the differential equations 1 and 2, considering as initial conditions an empty lattice, $\rho_i^0 = 0, \quad i = 1, 2, ..., N$.

2 Implementation of the code

I will reproduce the dynamics through an agent based model. In my simulation, I consider a one lane road as the one dimensional lattice. It is composed, on the x axis, of 101 sites of the lattice (that are called *patches* on NetLogo and that constitute its environment). The cars are injected on the road with rate *alpha* and exctracted with rate *beta* and can move rightward if the adjacent patch is empty. I want to reproduce the density profile of the sites: an occupation number ($n_i^t = 0, 1$) is assigned to each patch. Thanks to this parameter, I define the local density ($\rho_i^t = \langle n_i^t \rangle$) of each patch as the temporal mean of its occupation number in the time interval considered, and then I plot the value of the density for all the patches at each time.

2.1 Interface of the simulation

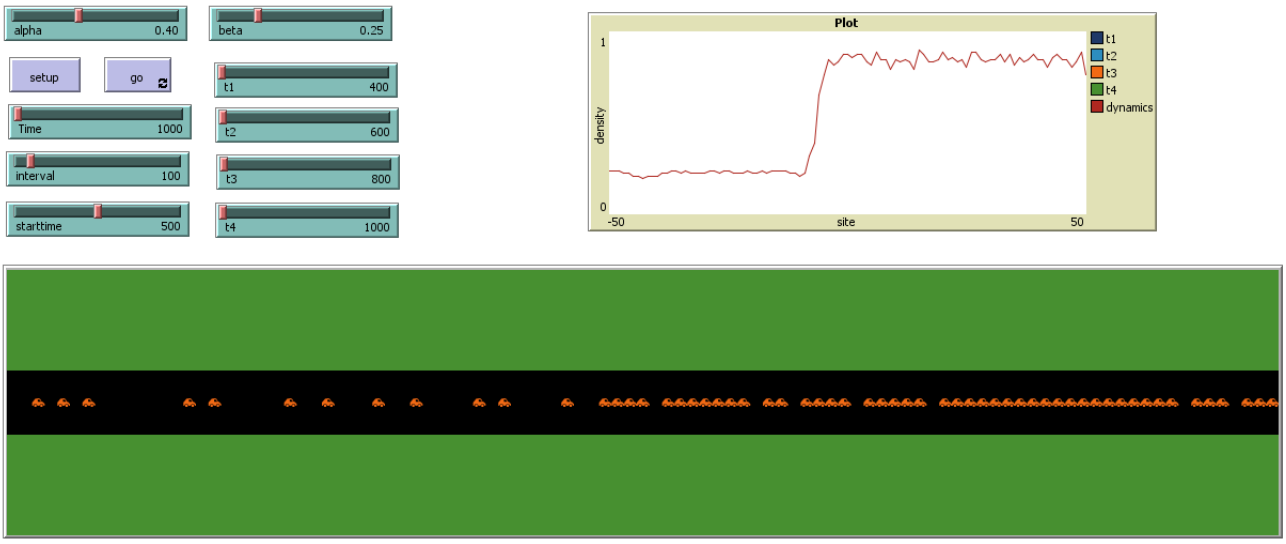

Figure 7: Interface of the NetLogo simulation

As figure 7 shows, there are two buttons (*setup* and *go*), and some sliders in the interface. The sliders *alpha* and *beta* rule the input and extraction rates of the cars, and enable an analysis of the different phases of the model. The slider *Time* regulates the time after which the user wants the simulation to stop: it is connected to the time after which it is known that a stationary state is reached. There is also the slider *starttime*: the user can choose to wait a transitory time before starting the calculus of the densities, and the value of this slider is updated during the simulation if *interval* is set to a non zero value. The slider *interval* defines the time interval in which the user wants to consider the occupation numbers of each node to calculate the respective density, that is the interval in which you assume that the occupation numbers of each node are correlated in time.

Then there are four sliders, *t1*, *t2*, *t3*, *t4*, that fix four values of time on which the user wants to focus: the values of the densities corresponding to these times are stored and plotted together at the end of the simulation.

2.2 Netlogo procedures

2.2.1 The setup button

The *setup* command clears the environment, sets the shapes of the *turtles* (the agents) to cars, initializes the variables, and creates a one-lane road, black-coloured, sorrounded by a green environment.

```
to setup
  clear-all
  set-default-shape cars "car"
  ask patches [
    ifelse abs pycor < 3
      [ set pcolor black]
      [ set pcolor green  - 1]
  ]
  ask patches [set history[] ]
  set densities[]
  set list1 []
  set list2 []
  set list3 []
  set list4 []
  set sites patches with [abs pycor < 1]
  set xsites [pxcor] of patches with [abs pycor < 1]
  set starttime 0
  reset-ticks

end
```

2.2.2 Movement procedures

I will now show some functions that are present in the main button of the simulation, the *go* button, which performs the action.

```
to move
  ask cars[
    ifelse pxcor = 50 [fd 0][if not any? turtles-on patch (pxcor + 1) pycor [fd 1]]
  ]

end

to make-new-car [ freq x y h ]
  if (random-float 1 < freq) and (opz) [
    create-cars 1 [
      setxy x y
      set heading h
      set color orange
  ]]
end

to extract-a-car [ freq x y ]
  if (random-float 1 < freq) and (opz2)
    [ask cars-on patch x y [die]]
end
```

The functions *make-new-car* and *extract-a-car* are responsible for the injection and exctraction of cars at precise rates. They are excecuted if the global variables respectively *opz* and *opz2* are True, which I will explain in paragraph 2.2.3.

The *move* function makes cars move one step forward, provided the adjacent patch is empty, and provided the car is not on the last patch, where indeed its movement must be controlled by the *extract-a-car* function (the environment is indeed a torus, and without this specification a car on the last patch would continue its movement on the first patch).

2.2.3 The go button

```
to go
  if ticks > Time [unique-plot
    stop]

  ifelse not any? turtles-on patch -50 0 [set opz True][set opz False]
  ifelse any? turtles-on patch 50 0 [set opz2 True][set opz2 False]

  move
  extract-a-car beta 50 0
  make-new-car alpha -50 0 90

  if ticks > starttime [
      set densities[]
      foreach sort sites[[p] -> ask p [ ifelse any? turtles-on patch pxcor pycor
      [set occnumber 1.][set occnumber 0.]
      set history lput occnumber history
      set density mean history
      set densities lput density densities]]
      plot-dens]


  if ticks = starttime + interval[
    ask patches [set history[]]
    set starttime starttime + interval]

  if ticks = t1 [ set list1 densities]
  if ticks = t2 [ set list2 densities]
  if ticks = t3 [ set list3 densities]
  if ticks = t4 [ set list4 densities]

  tick
end
```

The *go* button is responsible for the action, which proceeds until the *Ticks* overcome a fixed value *Time*. The two ifelse-loops are fundamental for the execution of the *make-new-car* and *extract-a-car* functions. These lines let the cars behave actually as *Cellular automata*: in this model it is necessary that at each time t each cell (here patch) checks its state and the states of its neighbours, in order to change its state at time $t + 1$, simoultaneously with all the other cells, on the base of fixed rules (here defined by the functions *make-new-car*, *extract-a-car* and *move*). Thanks to this lines of code firstly the states of the patches are checked, and then all the actions are performed together and do not interfere. Then the *go* button calls the movement functions. In the next part of

the code, a loop over the patches of the 1-D lattice (*sites*) is done, in order to assign an occupation number variable to each site, which, as I have said in the introduction, is equal to 1 if the patch has a car on it or equal to 0 otherwise. A list *history* belongs to each patch, and is filled at each time with the *occnumber* value of that site. Lists that contain the memory of the occupation numbers are so created, and then a mean is taken for each list, in order to obtain an expected value (*density*, what I have called in the theoretical introduction ρ_i^t) for each patch. Then every *density* is added to a list *densities* that will enable the density plot next, which is driven by the function *plot-dens*. The next if-loop is excecuted when the variable *interval* is set to a non zero value. Finally, the last if-loops create four lists, in which the values of the densities at the times selected through the sliders *t1*, *t2*, *t3*, *t4* are stored.

2.2.4 The plots

The *plot-dens* function plots the values of the list *densities* versus the corresponding abscissa of the site, and shows the density profile. It is executed at each time, so a dynamic plot is obtained.

```
to plot-dens
  clear-plot
  set-current-plot "Plot"
  set-current-plot-pen "dynamics"
  let v 0
  while [v < length densities][
    plotxy item v sort xsites item v densities
    set v v + 1]
end
```

Finally, the function unique-plot is executed at the end of the simulation, and plots together the values of the densities stored in the lists *list1*, *list2*, *list3*, *list4* versus the abscissa of the sites.

```
to unique-plot

  clear-plot
  set-current-plot "Plot"
  set-current-plot-pen "t1"
  let a 0
  while [a < length list1][
    plotxy item a sort xsites item a list1
    set a a + 1]

  set-current-plot-pen "t2"
  let b 0
  while [b < length list2][
    plotxy item b sort xsites item b list2
    set b b + 1]

  set-current-plot-pen "t3"
  let c 0
  while [c < length list3][
    plotxy item c sort xsites item c list3
    set c c + 1]

  set-current-plot-pen "t4"
  let d 0
  while [d < length list4][
    plotxy item d sort xsites item d list4
    set d d + 1]

end
```

3 Results of the simulation and comparison with the theoretical expected results

I will now compare the expected dynamics of the theoretical model with the results of my simulation. I will explore the evolution toward the stationary state in the various phases, I will distinguish $\beta < \frac{1}{2}$ and $\beta > \frac{1}{2}$ and in both cases I will consider increasing values of α. I will start my analysis setting the value of *starttime* and *interval* to zero in the simulation.

3.1 Case of $\beta < \frac{1}{2}$ and $\alpha < \beta$

I will start with $\beta < \frac{1}{2}$ and $\alpha < \beta$. For these values of parameters, the stationary state is in the low-density phase. In figures 8 and 9 I report the density profile, at various times, for $\alpha = 0.2$ and $\beta = 0.25$, as expected by the theoretical model and as obtained from the simulation. From Figure 8 it is possible to see that particles entering from the left create, at short times, a region of constant density α. Eventually, the rightmost particles will hit the right boundary, creating a small "traffic jam". The result is a so-called *shock* profile, where the density increases sharply toward the value $1 - \beta$ corresponding to the right resevoir. This is in line with the simulation, where it is also possibile to see that the shock remains confined to the right boundary, since its velocity is positive. Indeed, it can be shown that a shock between two regions of densities $\rho_L = \alpha$ and $\rho_R = 1 - \beta$ moves with velocity $v_s = \beta - \alpha$, that is indeed positive in this case. The profile shown in both figures for $t = 200$ is indistinguishable from the stationary state profile.

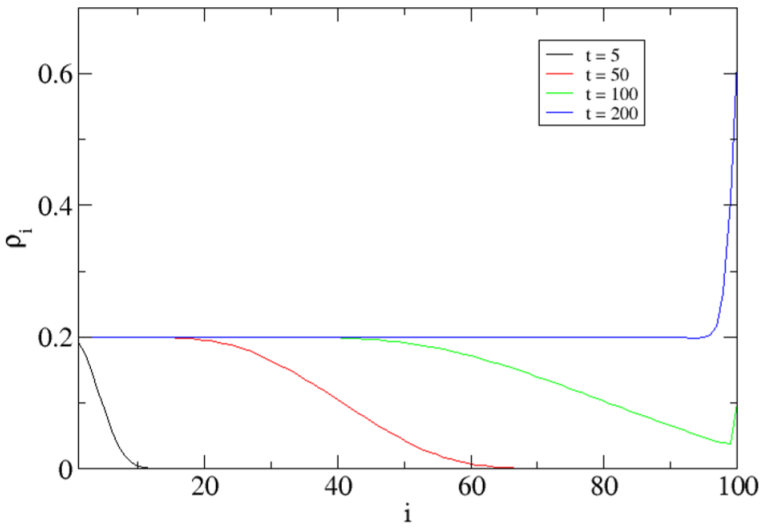

Figure 8

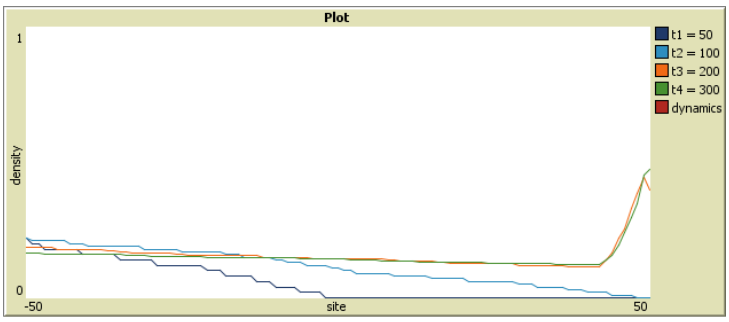

Figure 9: Density profile from the simulation for $\alpha = 0.2$ and $\beta = 0.25$, when the stationary state is in the low density phase: it is possible to see that after a time $t \approx 300$ the density reaches a bulk value $\rho = \alpha = 0.2$, which extends to the left boundary.

3.2 Case of $\beta < \frac{1}{2}$ and $\alpha = \beta$

Let us now increase α to the value $\alpha = \beta$, where the stationary state is at coexistence between a low-density and a high-density phase. In figures 10 and 11 I report the theoretical density profile and the one obtained from the simulation, at various time, for $\alpha = \beta = 0.25$. For these values of parameters, the evolution takes place in a longer time than in the previous case. Because of this, it is useful to set the slider *interval* in the simulation to a non-zero value, in order to see better the "instant" evolution of the densities, considering a smaller number of occupation numbers (in the hundreds) as correlated in time. Here I set *interval* to 100.

From 10 it is possible to see that now the shock, whose velocity $v_s = \beta - \alpha$ is expected

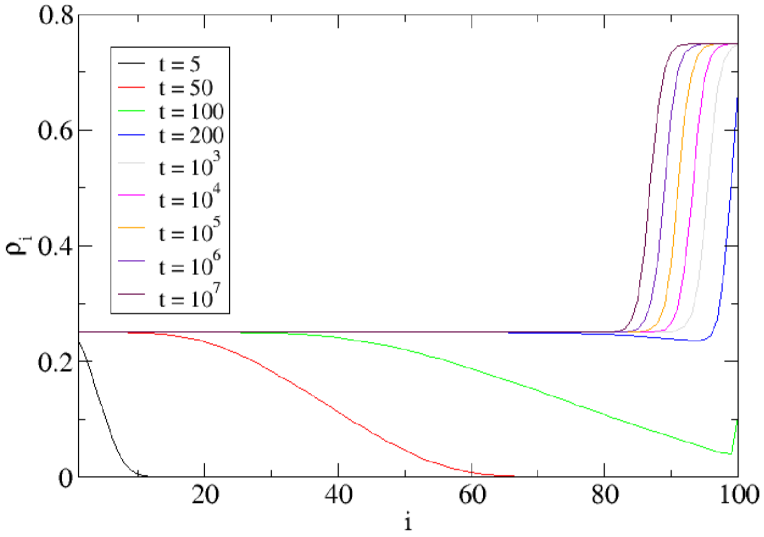

Figure 10

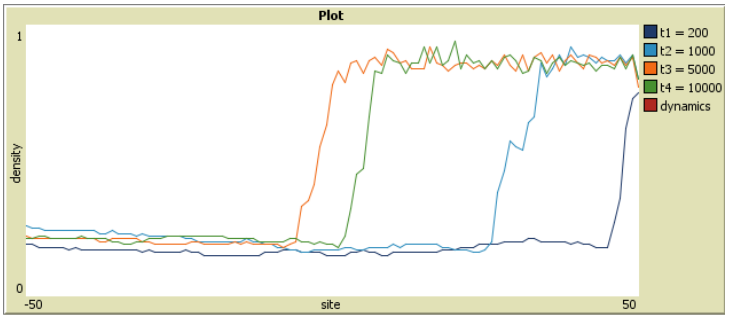

Figure 11: Density profile from the simulation for $\alpha = \beta = 0.25$, when the stationary state is at the coexistence line. It is possible to see the formation of two bulk densities, $\rho_L = \alpha = 0.25$ which extends to the left boundary and $\rho_R = 1 - \beta = 0.75$ which extends to the right boundary, that are separated by a *shock* or *domain wall*, whose position is affected by finite size effects.

to vanish, moves very slowly (logarithmically in time) towards the center of the lattice. This is a finite size effect. In 11 it possible to see that as expected two bulk densities appear. However, figure 11 shows that many fluctuations affect the position of the shock: its position could actually be anywhere, since, even if it seems to move to the left boundary, it could happen that it moves back closer to the right boundary at some times, as it happens at $t = 10000$. This can be due to the fact that in this phase the position of the shock is affected by finite size effects. Indeed, in the limit of $N \to \infty$, the domain wall can be anywhere: an infinite number of solutions appears, whose average gives a linear profile, as it is possible to see from the exact solution in figure 4. Setting back the slider

to zero and considering a mean over the occupation numbers that takes into account all the time, a linear profile seems to appear (Figure 12), which is indeed in line with the exact solution expected.

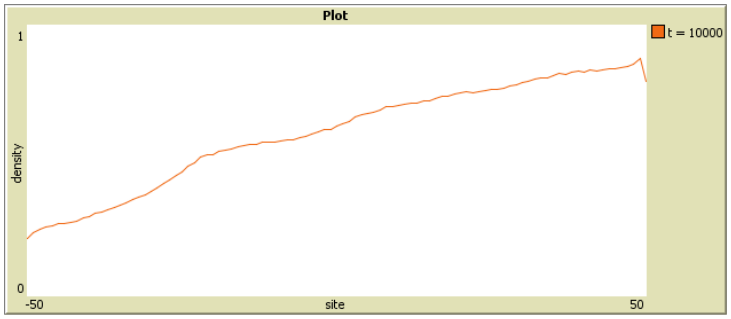

Figure 12

3.3 Case of $\beta < \frac{1}{2}$ and $\alpha \in (\beta, \alpha_c(\beta))$

We can now increase α to a value $\alpha \in (\beta, \alpha_c(\beta))$, where the stationary state is in the high-density phase and α is under a critical threshold $\alpha_c(\beta)$ such that the relaxation rate depends on α in this range. In figures 13 and 14 I report the density profile expected by the theoretical model and the one obtained from my simulation, at various times, for $\alpha = 0.4$ and $\beta = 0.25$. Here I set, as in the previous case, the value of *interval* to 100.

The shock, whose velocity $v_S = \beta - \alpha$ is now negative, moves to the left until it reaches the left boundary. The dynamics converges to the high density phase, with a bulk density $\rho = 1 - \beta$. My simulation shows this behaviour too, and the characteristic times are in a good accordance with the theoretical previsions: in both figures the profile for $t = 1000$ is indistinguishable from the stationary state profile.

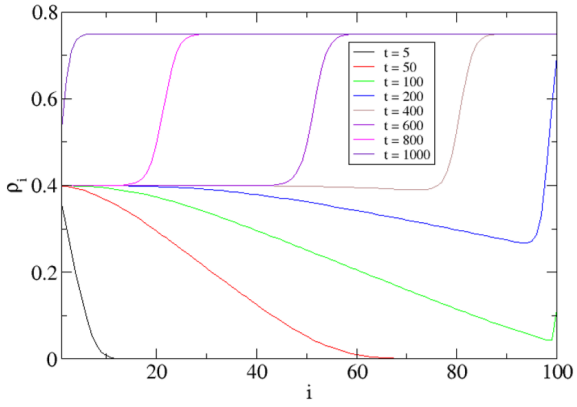

Figure 13

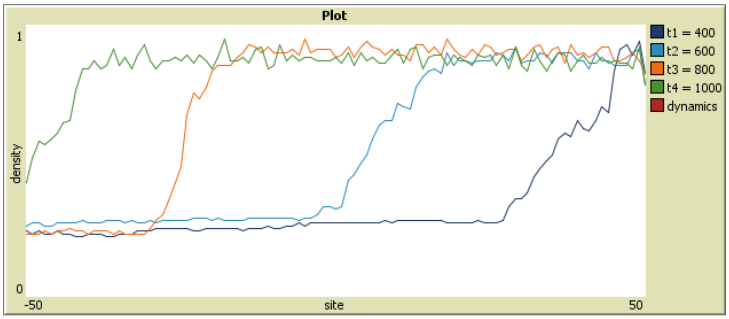

Figure 14: Density profile for $\alpha = 0.4$ and $\beta = 0.25$, when the stationary state is in the high density phase. It is possible to see that after a time $t \approx 1000$ the density reaches a bulk value $\rho = 1 - \beta \approx 0.75$ which extends to the right boundary.

3.4 Case of $\beta < \frac{1}{2}$ and $\alpha > \alpha_c(\beta)$

I conclude the discussion of the case $\beta < \frac{1}{2}$ by increasing further α to a value $\alpha > \alpha_c(\beta)$, where the stationary state is still in the high-density phase and the relaxation rate is now independent of α. In the figure below I report the density profile for $\alpha = 0.6$ and $\beta = 0.25$. I set in this case *interval* to 120.

As figure 15 shows, at odds with the previous cases, on the left of the shock the density profile is not anymore constant and equal to α, the limiting density close to the shock is smaller than α. Figure 16 confirms that the shock still moves forward the left boundary, and that the density on the left of the shock is not anymore constant and equal to α, even if this is evident only in the earlier stages of the simulation. Moreover, in this case it seems that the dynamics of the simulation is a little faster than the one predicted. Repeating this analysis, now setting instead *interval* to zero, the possibility to see in details the evolution of the shock is lost, but a better view of the non costant nature of the density on the left of the shock is gained, as figure 17 shows.

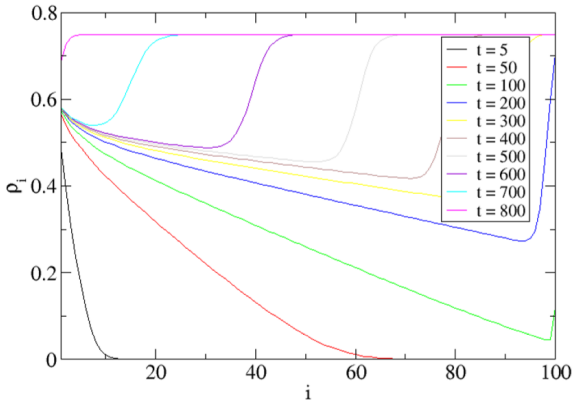

Figure 15

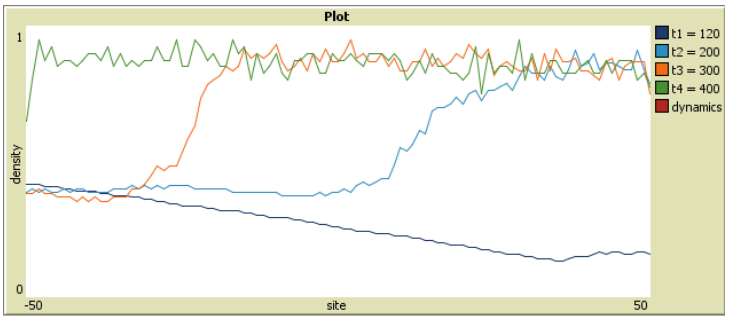

Figure 16: Density profile from the simulation, when the stationary state is in the high density phase, for $\alpha = 0.6$ and $\beta = 0.25$.

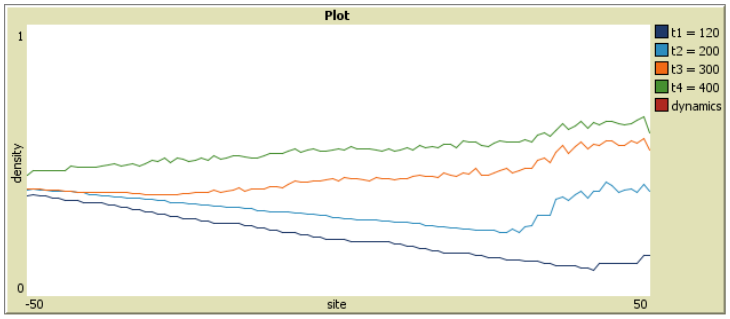

Figure 17: Density profile from the simulation, when the stationary state is in the high density phase, for $\alpha = 0.6$ and $\beta = 0.25$, obtained setting *interval* to zero: it is possibile to notice that the density on the left of the shock is not anymore constant.

3.5 Case of $\beta > \frac{1}{2}$ and $\alpha > \frac{1}{2}$

I will now turn my attention to the case $\beta > \frac{1}{2}$. As far as $\alpha < \frac{1}{2}$ the stationary state is in the low-density phase and the dynamics is qualitatively similar to the one seen at $\beta < \frac{1}{2}$.

A dynamical transition in encountered upon increasing β above a critical threshold, with features that are symmetric to those characterizing the high-density phase. Let us now increase α to a value $\alpha > \frac{1}{2}$, where the stationary state is in the maximal current phase. In the figure below I report the density profile, at various times, for $\alpha = \beta = 1$. For this last analysis I set back *interval* to a zero value.

From both 18 and 19 it is evident that no shocks are present, and that the relaxation towards the stationary state is much slower than in the other phases. The density profile at $t = 10000$ is in both figure indistinguishable from the stationary one. At that time it is possible to see in both figures that the density assumes a central bulk value equal to 0.5: the current, that, when a bulk solution of the density is reached, is given by the formula $J = \rho(1 - \rho)$, assumes the maximum possible value, $\frac{1}{4}$. The current is indeed optimized in this phase, and, for these particular values of $\alpha = \beta = 1$, the dynamic is trivial: the particles are injected and extracted with probability equal to 1, the dynamics is so deterministic and the particles do not create traffic jams, as Figure 20 shows.

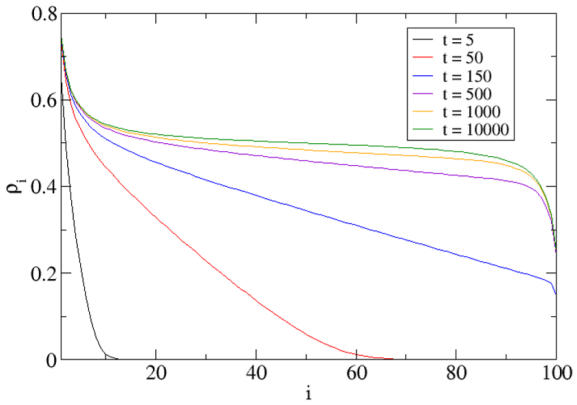

Figure 18

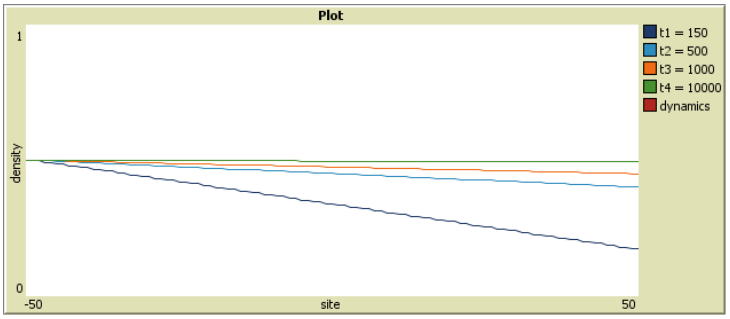

Figure 19: Density profile from the simulation fo $\alpha = \beta = 1$, when the stationary state is in the maximal current phase.

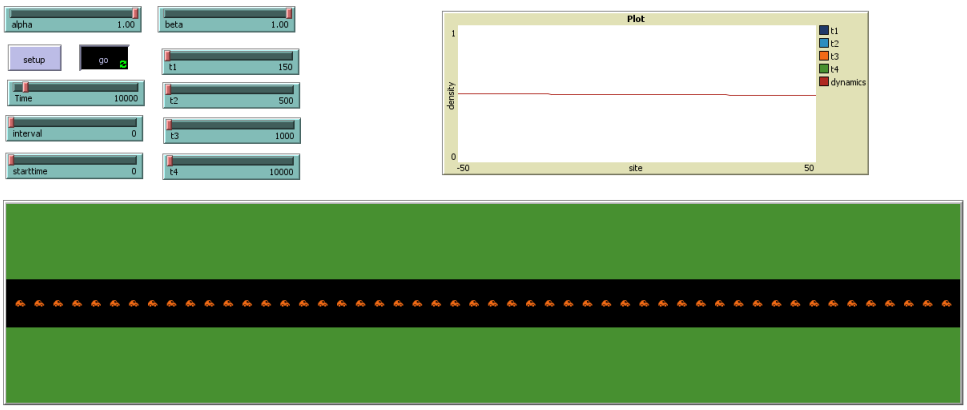

Figure 20: Setup of the NetLogo interface in the maximal current phase, in particular when $\alpha = \beta = 1$. It is easy to see that the current is optimized.

4 Conclusions

I can say that the simulation reaches a good accordance with the theory: some differences from the theoretical configurations (that I have found, for example, in paragraph 3.4 as regard the characteristic times) can be accepted since many different realizations may conduct to the same stationary state. Indeed, unlike the theoretical model, where the set of differential equations 1 and 2 has precise initial conditions and so unique solutions, here the parameters α and β, when different from 1, insert a stochastic component in the model out of the stationary state.
Moreover, the accordance is good considering my definition of densities: in the theoretical model, the densities are the result of a recursion relation in the case of the stationary state, and of a set of differential equations out of the stationary state. They are so uniquely defined by mathematical relations, and no possible implementations are suggested in the theoretical model. My definition is biased by the slider *interval*, which I set to non-zero values when I considered it reasonable.
Finally, I have to remark the assumptions I made deriving the theoretical model. I firstly assumed mean-field, which is actually a crude assumption. As regard the stationary state, I assumed that at a certain time the observables would not depend on time. Moreover, as regard the bulk solutions, I assumed that the model can exhibit them in the large N limit and sufficiently far from the boundaries. Despite these assumptions, that my simulation does not exploit, the results of the dynamics are in line with the theoretical expected ones and there is a great accordance with the bulk solutions of the expected stationary state. This could show the robustness of the theoretical model, which seems to work for finite size systems too.

References

[1] J.H. Gibbs C.T. MacDonald and A.C. Pipkin. *Biopolymers*, 6:1, 1968.

[2] J.H. Gibbs C.T. MacDonald and A.C. Pipkin. *Biopolymers*, 7:707, 1969.

[3] Alessandro Pelizzola (lecture notes of the course of Biophysics at Politecnico di Torino). *Biophysics (Statistical physics of biopolymers)*. 2017-2018.