EGGTART: User Manual

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1 Introduction

This document is the EGGTART User Manual, giving an overview of the software's interactive features and how to run it.

1.1 What is EGGTART?

EGGTART (**E**xtensive **G**UI **g**ives **T**ASEP-realization in **r**eal-**t**ime) is a software package that provides a visualization of the dynamics associated with the generalized Totally Asymmetric Simple Exclusion Process (TASEP). The TASEP is a classical stochastic process (detailed in Section 3) which has been used to model transport phenomena in various non-equilibrium particle systems in statistical physics, traffic systems, and biology [1]. In the context of mRNA translation [2], we have recently studied [3, 4] a generalized version of the TASEP, called the inhomogeneous ℓ-TASEP. While the original TASEP model simply considers particles of size one and homogeneous hopping rates on a lattice, this generalized version takes into account the size of particles ℓ and inhomogeneities of the particle hopping rates.

Our theoretical results [4] provide analytic formulas for general statistics associated with the inhomogeneous ℓ-TASEP. These results have the advantage of enabling an immediate quantification of the process as a function of the different parameters associated with it, which is impossible to achieve via traditional stochastic simulations. More precisely, our methods rely on solving a non-linear PDE that generalizes the Burgers' equation and describes the average dynamics of the current. This PDE is derived from considering the process in its so-called "hydrodynamic limit", obtained as the lattice size gets large. For more details on the process and methods, we invite the user to read Section 3.

To help mathematicians, physicists and biologists visualize these results and apply them in other contexts, we have developed the present software, which provides a user-friendly and easy-to-run graphical user interface. For any values of particle size, entrance rate, exit rate, and site-specific hopping rates, EGGTART provides a complete visualization of the main quantities of interest of the process, such as the particle current, density, and a full description of the phase diagram associated with different types of particle traffic behavior. The scope of our visualization might be of interest not only to researchers primarily studying interacting particle systems, but also mathematicians and physicists working on PDEs, as it leads to identify major shocks, rarefaction waves and ultimately the stationary density achieved in the long-time limit for a general conservation law.

1.2 Development and hardware requirements

EGGTART has been developed in Python 3.6. It uses the packages `numpy` and `pyqtgraph`, which requires `pyqt4` or `pyqt5`. For ease of installation, we provide an executable version of the software that does not require having Python and the required add-on packages installed. We provide different versions of EGGTART for Mac OS X, Linux (Ubuntu) and Windows (10). The software has been mainly tested on Mac. It works best with a scroll-wheel mouse.

1.3 Downloading and running EGGTART

EGGTART is available to download at the following address: https://github.com/songlab-cal/eggtart.

- **For Mac users:** Download `EGGTART.app.zip`. After unzipping it, open (use right click) the .app file.
- **For Ubuntu users:** Download `EGGTART`. Right click on the file; go to Properties, then Permissions and check "Allow executing file as program". Double click the file to run EGGTART.
- **For Windows users:** Download `EGGTART.exe`. Double click on the file, then click on "More info" and "Run anyway".

Running EGGTART should open the software main window.

2 General Features

2.1 Input file

EGGTART takes as main input a .csv file of numerical values, where the ith entry is the particle hopping rate at position i. The position is denoted by the variable x and the associated rate $\lambda(x)$. The lattice is normalized by the number of entries, such that $0 \leq x \leq 1$. To open an input file, use the *File* tab, then *Open*, or the keyboard command ⌘+o in the Mac version.

2.2 Exporting file

The figures displayed by the software can be exported in .png format, together with output variables in .csv format. To generate an output file, go to File › Export, or use the keyboard command ⌘+e in the Mac version.

2.3 General description of the interface

Loading the input file generates the default interface, which consists of six panels (see Figure 1) displaying the following:

1. particle hopping rate function λ,
2. parameters control panel,
3. ℓ-smoothed particle density ρ,
4. phase diagram,
5. current J and average density $\langle\rho\rangle_N = \frac{1}{N-\ell+1}\sum_{x=1}^{N-\ell+1}\rho(x)$ as a function of entrance rate α,

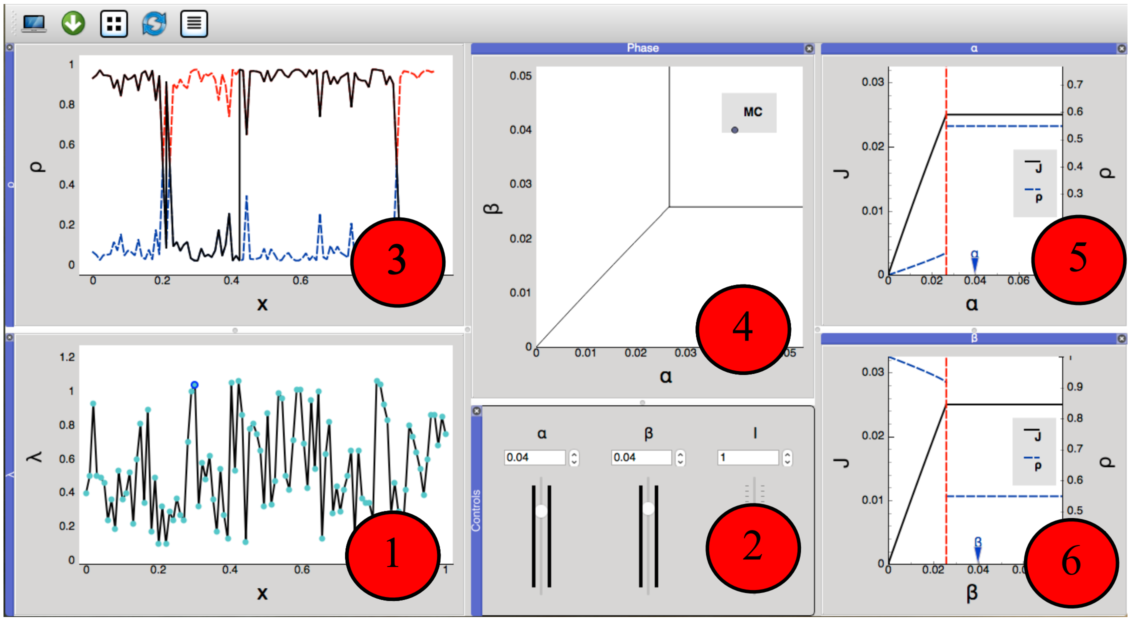


Figure 1: EGGTART default interface. The default interface generated after loading the input file is divided into 6 panels: 1) the particle hopping rates λ, 2) parameters control panel, 3) density plot ρ, 4) phase diagram, 5) current J as a function of entrance rate α, 6) current J as a function of exit rate β.

6. J and $\langle \rho \rangle_N$ as a function of exit rate β.

The layout of the panels can be modified and edited as follows:

- *Move panels*: Panels can be moved by using left click and dragging (click on the blue tab of the panel to be moved). Double click on the panel tab to get a floating panel.
- *Save and restore panel layout*: The icons at the top of the main window allow to (from left to right) restore the default panel layout, display/remove panel tab, save current layout, restore the saved layout and open/close specific panel windows.
- *Zoom in/out, center plots:* The plots in the panels can generally be modified using the mouse. Use the wheel mouse to rescale each axis (move the mouse on the side of the plot that needs to be rescaled). Left click and drag to recenter the plot.
- *Restore default view*: Right click on the plot to open a box asking to restore the original default view.
- *Change viewing range*: Right click on the plot, and click on 'View Range' to set the range of the viewbox.

2.4 Hopping rates

The hopping rates can be directly edited from the interface and the hopping rates panel (panel 1 in Figure 1) for direct visualization. There are two ways to modify a rate located by a small circle: Left click on a circle, and once it is emphasized in blue, click on it again and drag up and down to adjust the value. Alternately (for more precise specifications), right click on a circle. This opens an editing box where one can type a new value or use box arrows to change the rate value.

2.5 Control panel

Panel 2 in Figure 1 allows to modify the other parameters of the model by typing the desired value in the editing box or clicking on the box arrows:

- α is the particle entrance rate.
- β is the particle exit rate.
- ℓ is the particle size.

The parameters α and β can also be changed by dragging the ball in panel 4.

2.6 Particle density

For given values of the hopping rate function λ, entrance rate α, exit rate β and particle size ℓ (visualized in the λ and parameter control panels), panel 3 shows the resulting density plot function ρ (which approximates the ℓ-smoothed occupation measure, see Section 3.2). The red and blue lines indicate the upper and lower branch solutions (see Section 3). The physical density is plotted by the black curve.

2.7 Phase diagram

The phase diagram panel shows the different regimes of the phase diagram in α and β, separated by black lines (see Section 3). The ball indicates the current values of (α, β) from the parameters control panel, and the corresponding phase regime MC, LD (I or II) or HD (I or II) is displayed. The ball can be moved to modify the values of α and β (left click and drag).

2.8 Current visualization

The right panels in the default interface display plots of the particle current J and average particle density $\langle\rho\rangle_N$ over the whole lattice, as a function of α (panel 5) and β (panel 6). The values of α and β in the control panel are displayed by flags along the x-axis. The red line indicates the phase transition from LD to HD or MC for the α-panel, and HD to LD or MC for the β-panel.

3 Appendix

We provide here a brief description of the inhomogeneous ℓ-TASEP, its hydrodynamic limit and the associated phase diagram. For further details, see our paper [4].

3.1 The inhomogeneous ℓ-TASEP

The inhomogeneous ℓ-TASEP is an interacting particle system, where particles of size ℓ hop unidirectionally along a lattice of N sites under mutual exclusion: A particle at site $i \in \{1, \ldots, N\}$ remains put at i if the location ℓ sites ahead of it is occupied, and jumps at exponential rate p_i to position $i+1$ if site $i+\ell$ is empty. We here consider a system with open boundaries, where particles are continuously injected and ejected at rates α and β at the two lattice ends, a situation that is ubiquitous in diverse fields like molecular transport, gene expression, traffic flow and fluid dynamics [1]. Figure 2 provides a pictorial representation of this Markov process.

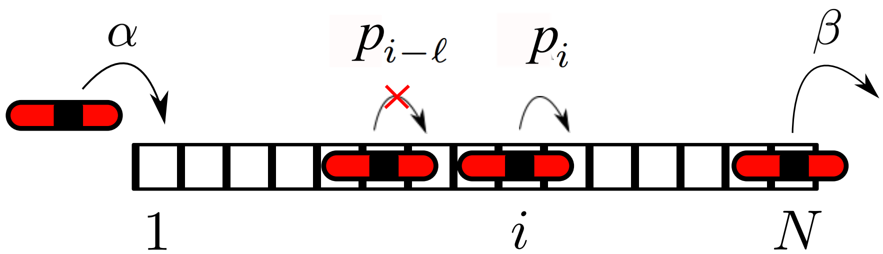


Figure 2: Illustration of the inhomogeneous ℓ-TASEP (taken from [4]) with open boundaries. Particles (of size $\ell = 3$ here) enter the first site of the lattice at rate α and a particle at position i (here denoted by the position of the midpoint of the particle) moves one site to the right at rate p_i, provided that the next ℓ sites are empty. A particle at the end of the lattice exits the lattice at rate β.

3.2 Hydrodynamic Limit

Although solving the inhomogeneous ℓ-TASEP is analytically intractable, this can be done in the continuum limit of the discrete process. More precisely, denoting by $\tau(t) \in \{0,1\}^N$ a particle-lattice configuration at time t, we showed that under Euler time scaling, the density of particles (i.e., the ℓ-smoothed occupation measure) $\rho(x,t)\mathrm{d}x = \lim_{N\to\infty} \frac{1}{N} \sum_{i=0}^{N-\ell+1} \frac{1}{\ell} \sum_{k=i}^{i+\ell-1} \tau_i(Nt)\delta_{\frac{i+k}{N}}(\mathrm{d}x)$ satisfies the inhomogeneous conservation law

$$\partial_t \rho = -\partial_x \left[\lambda(x)\rho\, G(\rho)\right] \tag{1}$$

where $G(\rho) = \dfrac{1-\ell\rho}{1-(\ell-1)\rho}$ and λ is a differentiable extension of $(p_1, \ldots, p_N)$, such that $\lambda(x) = p_{\lfloor Nx \rfloor}$.

For constant jump rates $\lambda \equiv p$ and particles of size $\ell = 1$, the hydrodynamic limit (1) reduces to the well-known one-dimensional Burgers' equation whose steady-state solutions are simply constants. Increasing ℓ and introducing spacial inhomogeneity generalizes this simple model substantially and leads to non-trivial solutions.

Finally, we emphasize that the hydrodynamic limit is only able to accurately predict *smoothed* particle profiles as made explicit in the definition of ρ. While this necessitates some care when working with, e.g., experimental data, which typically is generated in raw rather than smoothed form, the main determinants of transport efficiency depend on $\langle\tau\rangle_N$ solely through $\langle\rho\rangle_N$ and so no crucial information is lost when smoothing.

3.3 Phase diagram

3.3.1 Upper and lower branch solutions

Solving the characteristic equation associated with the hydrodynamic limit yields two general branches of solutions, both of which are displayed in panel 4 of the software. We call these two branches the upper (dotted red) and lower (dotted blue) branches. Choosing values for the parameters α, β imposes boundary conditions (depending on ℓ) that determine which branches are taken, leading to distinct regimes summarized by a phase diagram.

3.3.2 Phase diagram

The phase diagram in α and β consists of three regions:

1. Low Density (LD) phase: If α is small and β large, few particles enter the system while many leave for any fixed duration of time. This depletes the lattice of particles, makes collisions unlikely and establishes an overall density profile characterized by small occupation probabilities throughout the lattice. Such profile is associated with the *lower branch* of ρ.

2. High Density (HD) phase: Any low density branch of ρ has a dual profile of equal current that results from appropriately exchanging the roles of α and β, resulting in high lattice occupancy, large collision rates and consistently large densities. This dual profile is associated with the *upper branch* of ρ.

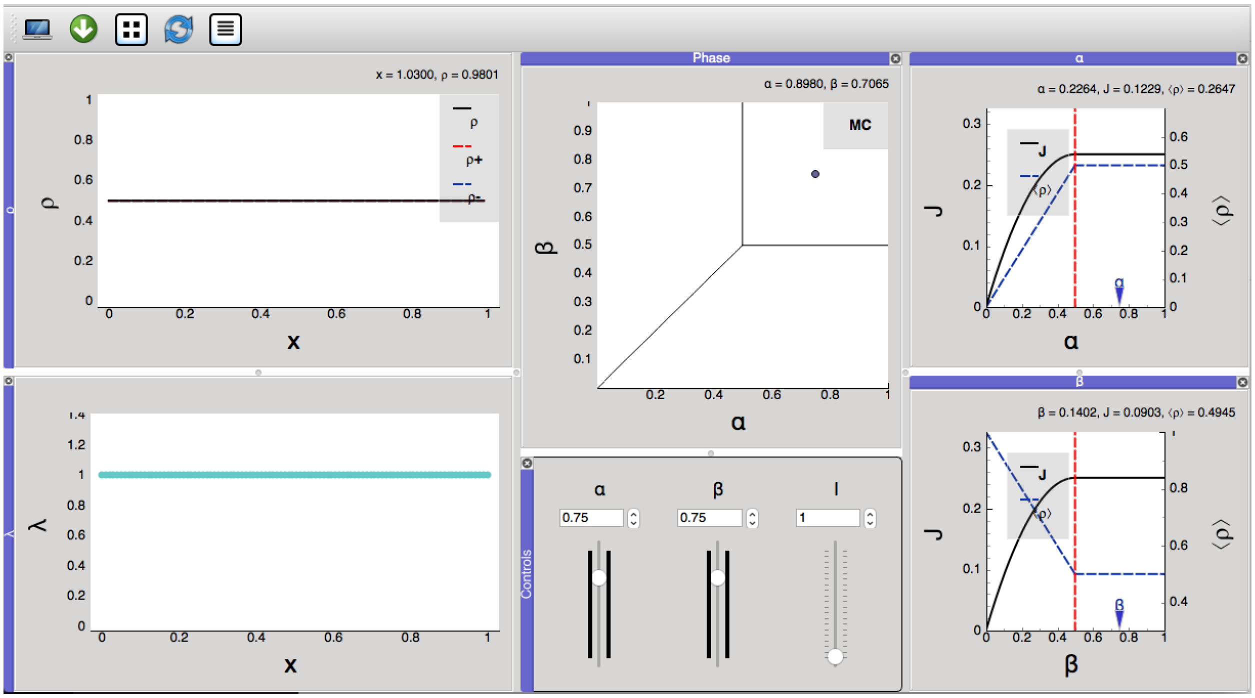
3. Maximum Current (MC) phase: When α and β both surpass system dependent thresholds, the current saturates at its maximal λ-dependent capacity, and a superposition of high and low density branches establishes itself at stationarity. The lattice site that separates high from low density is precisely the location of smallest speed.

Further stratification of LD and HD into classes I and II results from utilizing higher order information during the continuum scaling, and is important in applications sensitive to boundary behavior. Further information and details are given in [4].

4 Tutorial

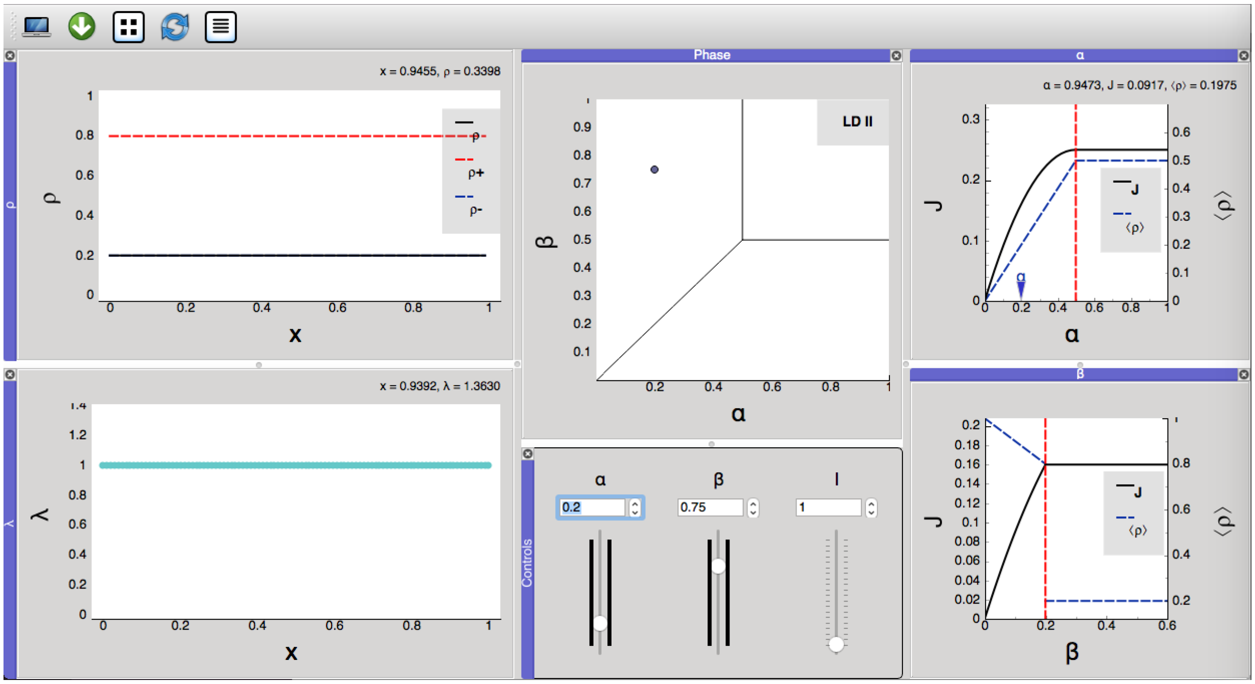
We provide here a simple tutorial to demonstrate the various features of EGGTART and the fundamental properties of the TASEP:

1. To begin with, let us visualize the original TASEP model. Load the input file called `homogeneous_rates.csv`:



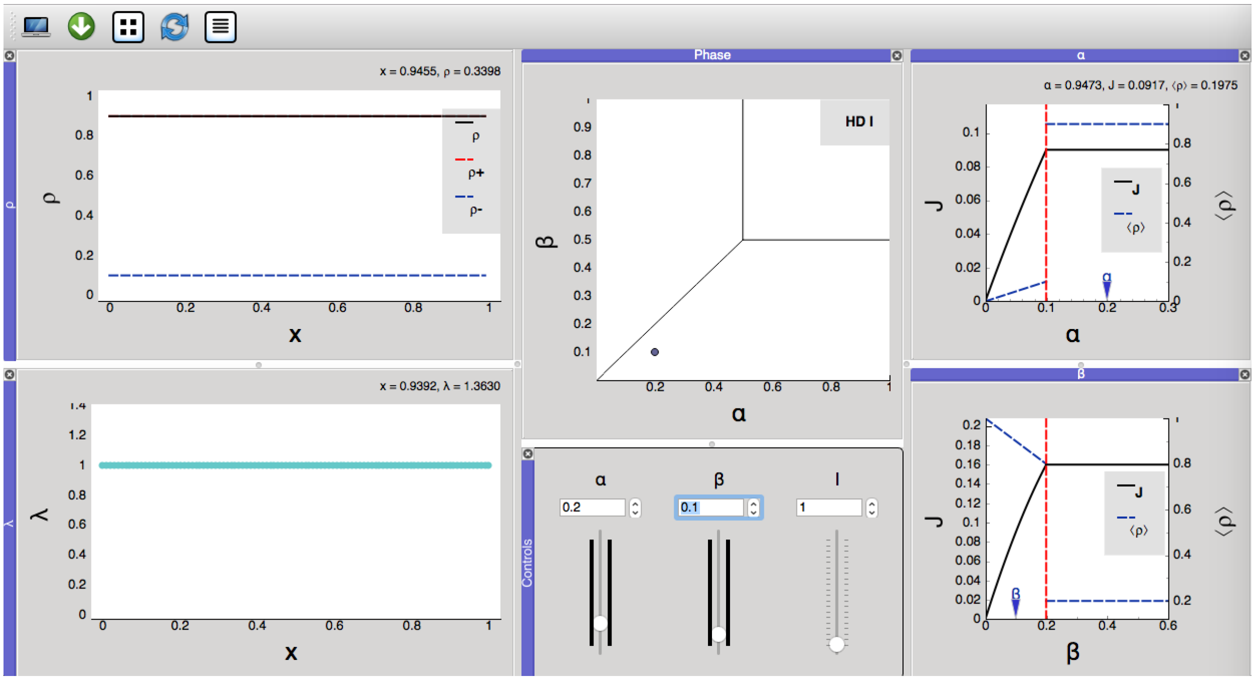
The λ panel (bottom left) displays the hopping rates. In the top left panel, you can visualize the bulk density. Default parameters α (entrance rate), β (exit rate) and ℓ (particle size) are displayed in the bottom middle panel. In the top middle panel, a ball indicates the current (α, β) in the phase diagram. One can see that the dynamics followed here is the MC (maximal current) regime, where both α and β are above their respective critical values associated with phase transitions (shown by red lines in the right panels). As the parameters are in the maximal current regime, one can also notice in the right panels that the current and average density are constant in this region.

2. Change the entrance rate α by typing a new value (0.2) in the left box located in the middle bottom panel (it is also possible to drag the ball located in the phase diagram):



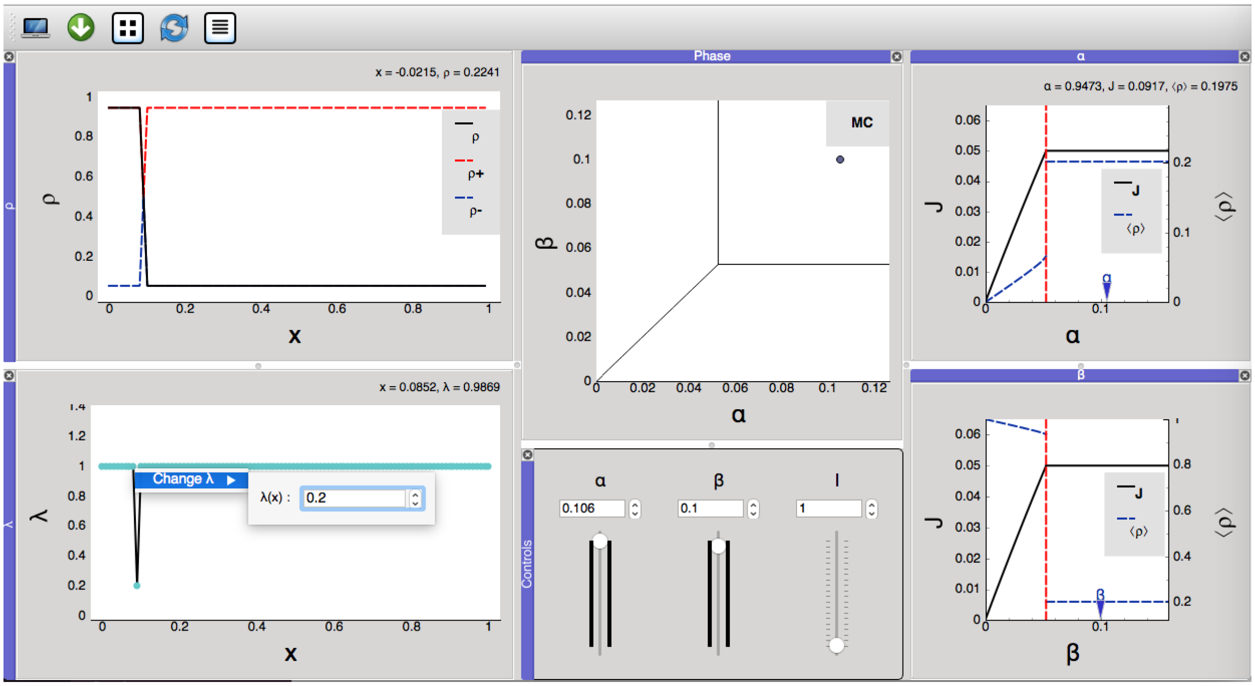
As a result, the ball in the phase diagram panel has now moved to the "LD" region and in the top right panel, the α flag is now on the left side of the critical red line. Instead of having a single branch of solutions, there are now in the ρ panel two branches, such that the solution of the hydrodynamic limit takes the lower one (with lower density).

3. To visualize the HD regime, modify β to 0.1 (same as in the previous step, with the middle box instead of the left one):



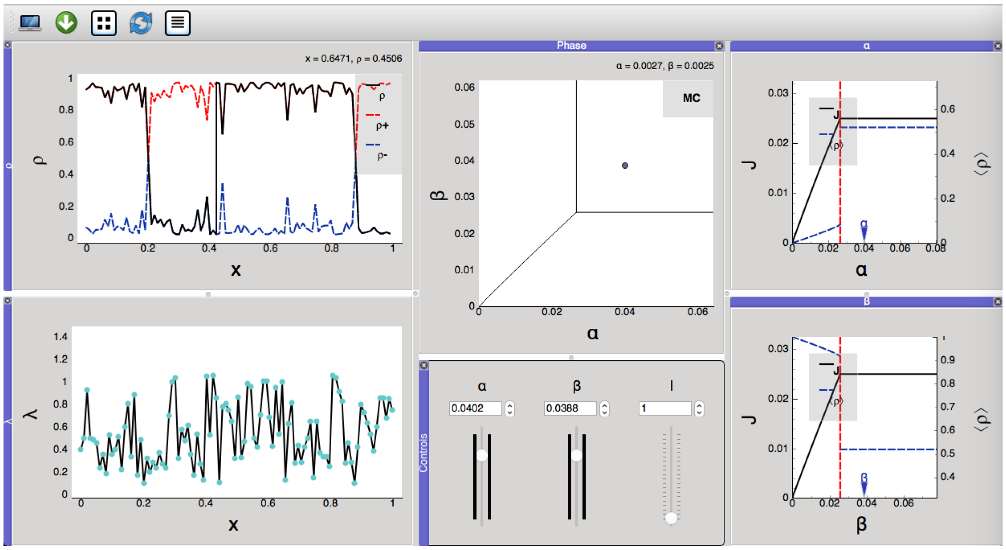
The density has now switched to the upper branch, while the position of β with respect to the critical line (shown in red) is reversed in the bottom right panel, and likewise for α in the top right panel.

4. We now introduce some “defect” in the rates. Right click on any point of the λ plot and decrease its value (e.g. 0.2):

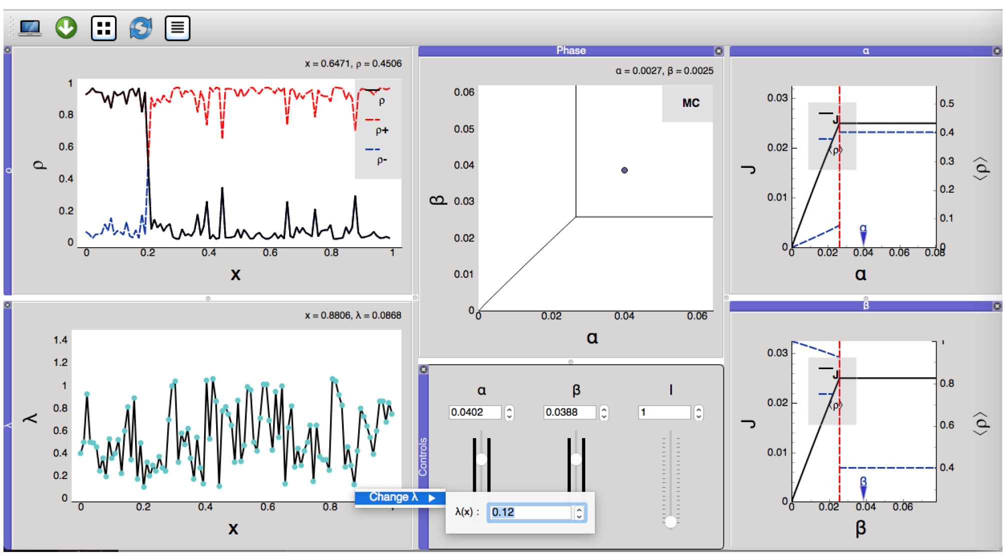


In the MC regime, one can now notice that two branches of solution co-exist, with ρ starting from the upper one before switching to the lower one at the defect location. Moreover, the range of J has decreased significantly.

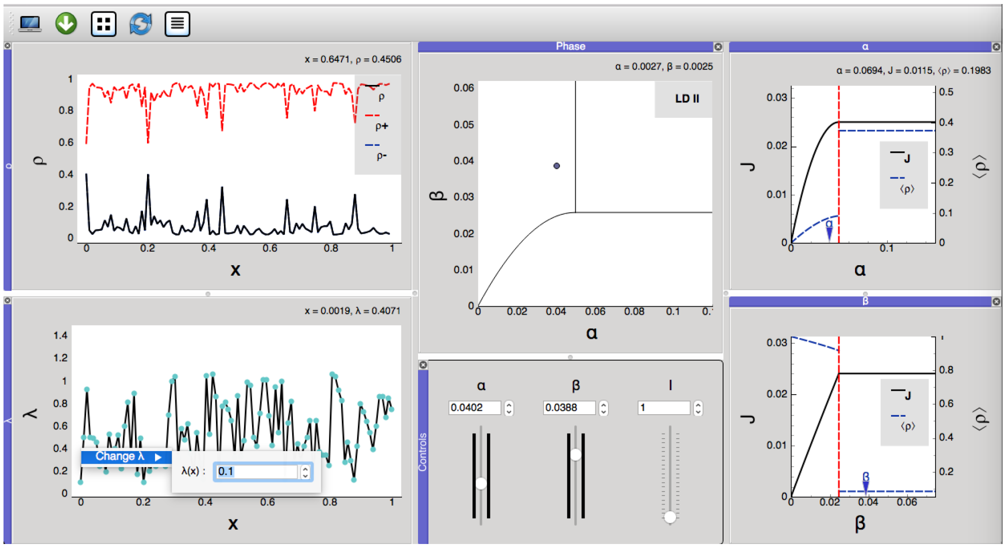
5. To visualize the impact of the rate heterogeneity, load the input file called `heterogeneous_rates.csv`:

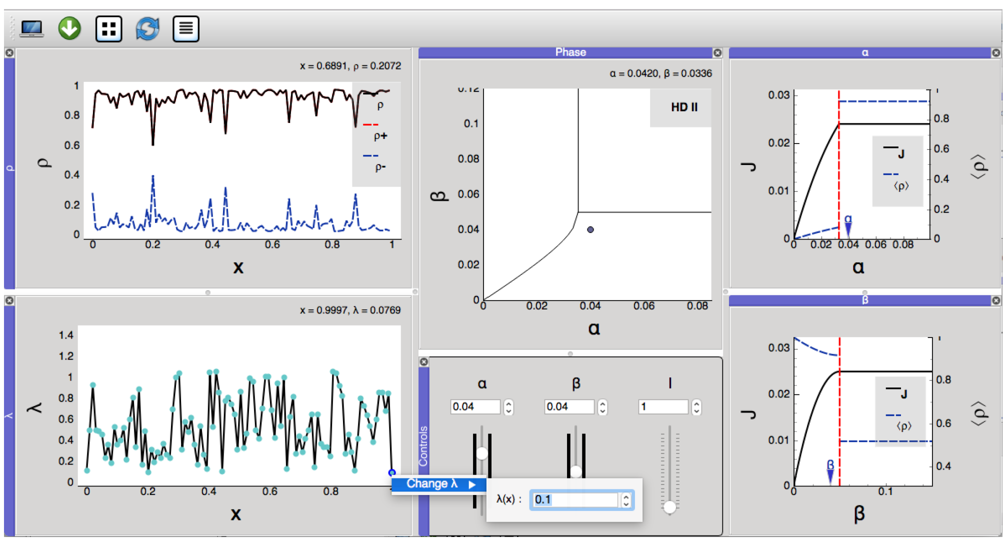


At positions where the hopping rate function λ achieves the minimum, the density switches between the two branches. Therefore, changing these locations can drastically affect the density over the whole lattice:

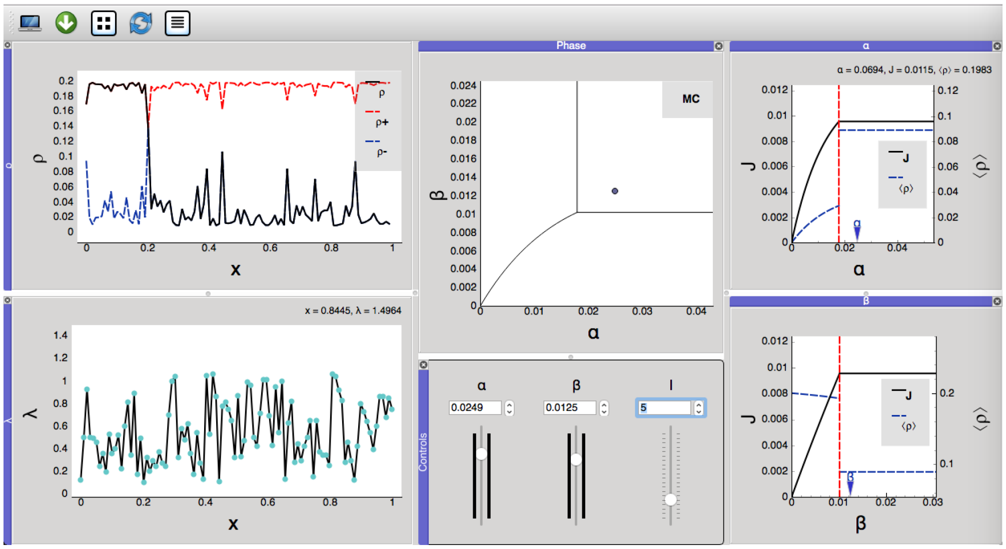


6. The phase transitions from LD to HD also depend on the value of λ at the boundaries of the lattice. By changing $\lambda(0)$ or $\lambda(1)$, one can notice that the separation between LD and HD in the phase diagram gets non-linear.





7. Finally, increase the value of the particle size ℓ to see how it decreases the density, current, and critical values of α and β, and also modifies the shape of the LD to HD phase separation:



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