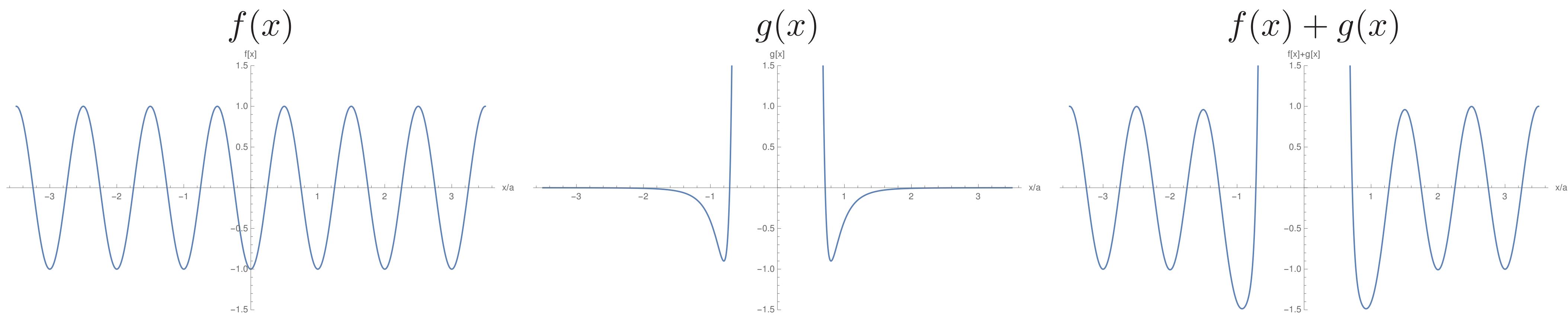
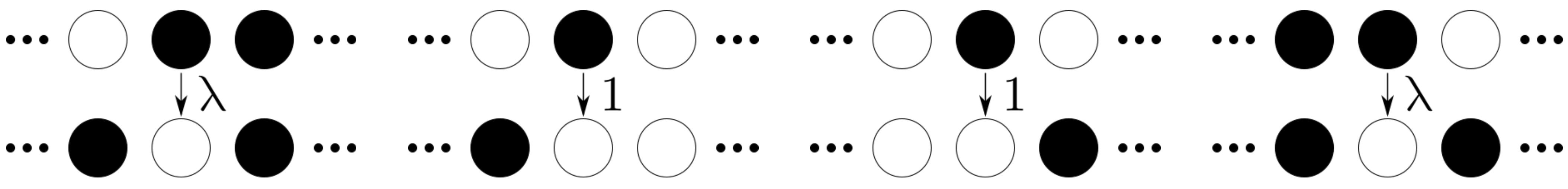


MODEL DEFINITION AND MOTIVATION

- Imagine many identical particles undergoing Brownian motion in a periodic potential with periodicity a . Perhaps this potential might look like the one portrayed by $f(x)$ as shown below.
- Let's now introduce interactions between these particles, consisting hard-core short range repulsion and slightly longer-ranged attraction, acting over a distance of $\mathcal{O}(a)$. Then if we were to place a particle at the origin, the potential felt by another particle would be like $g(x)$.
- Therefore the total potential experienced by a particle, the lattice potential plus the particle-particle interaction, would be $f(x) + g(x)$.



- The important thing to note here is that the main difference between the interacting ($f + g$) and noninteracting (only f) situations is that a particle wishing to escape the influence of an adjacent particle must jump over a taller potential barrier than it usually would. Observe also that only one particle may occupy a potential well at a time, due to the hard-core repulsion.
- This motivates us to define a model for particles hopping around on a 1D lattice, defined by the following allowed processes with their associated transition rates; black indicating occupation:



- More intuitively, particles hop into adjacent empty sites with rate 1 unless they have a particle already behind them, in which case they hop with rate λ ; the particles are "sticky" if $\lambda < 1$.
- The model I have described sounds pretty generic, and with good reason: this type of "sticky diffusion" behaviour happens in numerous situations. I originally made this model in order to investigate the growth of oxide layers on the surface of titanium, but it should be quite applicable whenever interacting entities attempt to diffuse through a lattice.

MODEL PHENOMENOLOGY

- The model described above obeys the detailed balance condition, and after a little relabelling can be shown to be equivalent to the Ising model in equilibrium.
- If we move our attention to the large-scale ($a \rightarrow 0$) limit and use mean-field theory, we may derive hydrodynamical equations that describe the current, J , of the particle density, ρ , like a fluid.
- In our model, the number of particles is conserved, so we have a continuity equation, $\partial_t \rho + \partial_x J = 0$.
- After a little mathematical effort, one may show that $J = -a [1 - (1 - \lambda)(4 - 3\rho)] \partial_x \rho$; current flows down the concentration gradient, in proportion to a coefficient $([\dots])$ which depends upon ρ .
- When $\lambda < \frac{1}{4}$, it becomes physically possible for that coefficient to be negative; thus, we have a prediction that sometimes particles might flow **towards** regions of higher concentration!
- This runs contrary to our usual intuition about how diffusive systems work...

NUMERICAL RESULTS

- Our continuum-limit mean-field theory has made some rather wild predictions about backwards diffusion; it would be nice if we had a way to test them.
- As luck would have it, the Kinetic Monte Carlo algorithm is ideal for simulating the kind of model we have described. It is implemented via Python-wrapped C++ in KMCLib[1].
- As of the time of writing, I have not yet confirmed or refuted the MFT current flow predictions. However, I have come across a variety of interesting behaviours exhibited by the model, and have included some images of them in the table below.

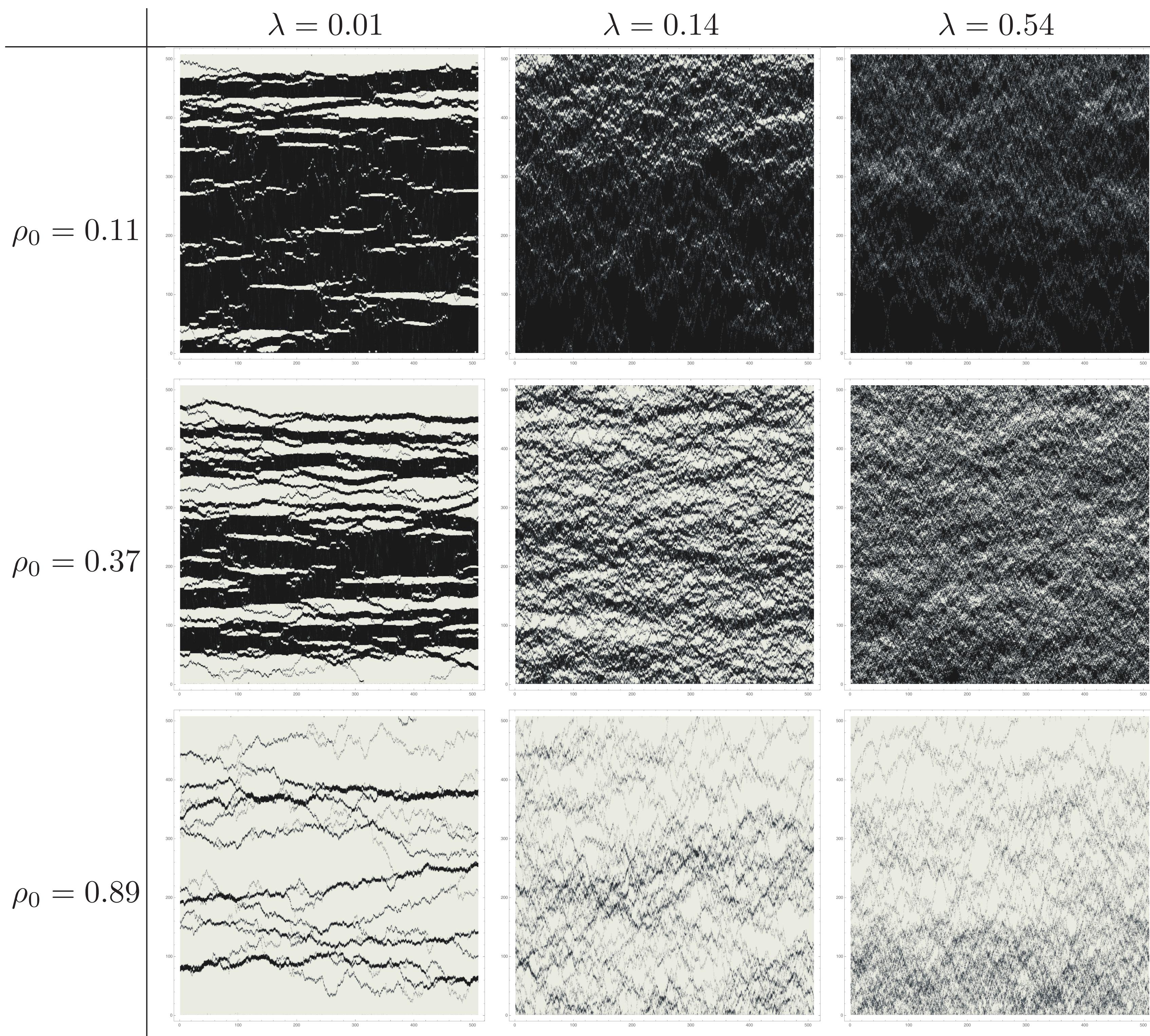


Table 1: The plots in this table display the particle density as a function of time and space, represented by the horizontal and vertical axes respectively; darker shades indicate lower density, lighter tones higher. In the simulation setup, the top boundary is maintained with $\rho = \rho_0 + 0.1$ and the bottom with $\rho = \rho_0 - 0.1$; hence under normal conditions, particles should on average flow from top to bottom.

CLOSING REMARKS

- I have recently started performing KMCLib calculations on the university cluster, Eddie. This should allow me to gather sufficient evidence about flow rates to be able to test our predictions.
- Once this 1D single-species model is properly understood, we can then think about generalising it to 3D or having multiple species.
- I would like to thank Graeme Ackland, Richard Blythe and Martin Evans for their help and guidance during this project, as well as my collaborator Mikael Leetmaa, the author of KMCLib.
- This research was funded by EPSRC with studentship grant number 1527137.