

Supporting Online Information: Implementation of the simulations

July 30, 2007

We have adapted the Gillespie algorithm for chemical reactions [1], which was originally thought for spatially homogeneous systems, to the case of particle transitions with spatio-temporal dependent rates. There are other existing Monte Carlo methods to perform the simulations (see e.g. [2]).

The system is characterized by a rate matrix $k_{i,j}$, where $i \in [0, N]$ specifies the site and $j \in [0, r - 1]$ the motor transition (r being the number of possible motor transitions; $r = 5$ in the present case). We order the transitions as follows: $k_{i,0} = k_f(i)$, $k_{i,1} = k_u(i)$, and $k_{i,2} = k_b(i)$, $k_{i,3} = k_{i,4} = k_d(i)$. Note that the rate matrix does not contain information about the motors occupying the sites. In order to account for the actual potential transitions, we define a global array in the system, a_l , with $l \in [0, N r]$, that characterizes the rates of all possible potential transitions, and it is defined as the number of motors that can undergo a particular transition times the rate of that transition: $a_{i r} = n_b(i)k_{i,0}$, $a_{i r+1} = n_b(i)k_{i,1}$, $a_{i r+2} = n_u(i)k_{i,2}$, $a_{i r+3} = n_u(i)k_{i,3}$ and $a_{i r+4} = n_u(i)k_{i,4}$, where $n_b(i) \in [0, 1] \subset \mathbb{N}$ and $n_u(i) \in \mathbb{N}$ are, respectively, the number of bound and unbound motors at site i (occupation numbers). Once the potential transition rates are given, we define the global transition rate as

$$k_g \equiv \sum_{l=0}^{N r} a_l . \quad (1)$$

Unlike discrete-time Monte Carlo simulations, where the time step of the simulation is set *a priori*, here it is necessary to know the time Δt at which the next transition takes place. This time is a stochastic variable distributed exponentially with a characteristic time scale $1/k_g$. Note that this time does not specify a particular transition of a certain motor, but only determines how long we have to wait to see a motor (no matter which) performing a transition. The actual transition that takes place is a stochastic variable distributed uniformly and is calculated as follows. Generate a stochastic number y distributed uniformly in the range $[0, k_g]$ and define m as an integer number in the range $[0, N r]$. The value of m that specifies the transition that occurs is the largest

value of $m \in [0, N r]$ that fulfills the following inequality:

$$\sum_{l=0}^m a_l < y . \quad (2)$$

The actual site i at which the transition takes place and the particular transition j , are given respectively by the quotient and the remainder of m/r .

The simulation evolves as follows. The system is initialized in a configuration with an initial number M_i of consecutive bound motors, the first one defining the position of the very tip of the tube, so that the initial length of the tube N is $N = M_i$. Then, the rate matrix is calculated, and the array a_l is obtained from the system configuration and the rates. The value of the global transition rate k_g is calculated for the initial configuration. Then, the following steps are repeated until a maximal time t_{max} :

- (step 1) Determine the stochastic time Δt at which the next transition occurs, the site i at which the transition takes place and the actual transition j .
- (step 2) The transition is performed if allowed by excluded volume interactions and the time t is updated to $t + \Delta t$.
- (step 3) The transition rates $k_{i,j}$ are then updated with the new configuration.
- (step 4) The array a_j is updated with the new configuration and value for the rates.
- (step 5) The global transition rate k_g is updated.
- (step 6) Go back to step 1.

This part of the algorithm determines the transitions of the motors, given the rate matrix and a particular configuration, but does not specify the dynamics of tube growth. The dynamics of the tube is specified by the rates of the motors (and their force dependence), and by a set of special rules for the growth events, which are defined in the main text.

References

- [1] Gillespie DT (1976) *J Comp Phys* 22:403-434.
- [2] Newman MEJ, Barkema GT, *Monte Carlo Methods in Statistical Physics* (Clarendon Press, 1999).