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Short Communication

Random sequential adsorption of line segments: universal properties of mixtures in 1, 2 and 3D lattices

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Abstract. — Monte Carlo results are reported for a process of random sequential adsorption on two and three dimensional lattices, of line segments of two different lengths chosen with various probabilities. The jamming limit, when considered as a function of the segment lengths and of the probability, is found to have the same behaviour in both two and three dimensions as was observed in one dimension. In addition, the kinetics of the process exactly follows the laws found in the solvable one dimensional case, where the rate of late stage deposit is given by the shortest segment probability.

Recently there has been a renewal of interest in the random sequential adsorption (RSA) model, especially in the case of well-defined mixtures of deposited objects [1]. In particular, a model for the deposition of line segments of two different lengths, chosen with equal probabilities, has been numerically simulated on a square lattice [2]. In the mean time, a one dimensional analog of this model, generalized to any mixture, has been solved [1, 3], thus providing a useful guide for the study of this process in higher dimensions. Many features of the 1D exact solution [3] are indeed already present in the results reported for the 2D Monte Carlo experiment of reference [2].

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The purpose of the present work is to generalize the numerical simulation of reference [2], to the case of arbitrary mixtures in two and three dimensions, in order to check whether the main properties of the 1D model hold in larger dimensions.

The model is defined as follows: segments of given length are sequentially and randomly placed on a $D$-dimensional lattice according to the following rules:

i) randomly select the length of the segment among two predefined values $l_1$ and $l_2 > l_1$ (measured in number of lattice sites), with probability $\alpha$ for the value $l_1$;

ii) randomly select a site on the lattice and a direction along one of the axes;

iii) if the selected site is empty, try to put the segment on the lattice along the selected direction with its origin on the selected site;

iv) if the segment can be placed such that it does not overlap previously deposited segments, it is left at this position and the attempt is successful;

v) if the selected site is occupied, or if there is no place for the deposited segment, the segment is withdrawn and the attempt is unsuccessful;

vi) whether or not the attempt is successful, the time counter is increased by $\delta t$ and a new try is realized.

The observable quantity of interest is the coverage $\theta(t; l_1, l_2, \alpha)$, defined as the fraction of sites covered by the deposited segments after a time $t$. This function has an infinite time limit, the jamming limit $\theta_\infty(l_1, l_2, \alpha)$, which, from the exact solution of reference [3], has the following properties in one dimension:

- for $l_1$ and $\alpha$ fixed it is an increasing function of $l_2$
- for $l_2$ and $\alpha$ fixed it is a decreasing function of $l_1$
- for $l_1$ and $l_2$ fixed it is a decreasing function of $\alpha$
- this last property leads to the discontinuous behaviour:

$$\theta_\infty(l_2) = \theta_\infty(l_1, l_2, \alpha = 0) < \lim_{\alpha \to 0} \theta_\infty(l_1, l_2, \alpha)$$

Furthermore, the jamming limit is approached exponentially with a rate simply related to the probability $\alpha$ and independent of the lengths $l_1$ and $l_2$:

$$\theta(t; l_1, l_2, \alpha) = \theta_\infty(l_1, l_2, \alpha) - C(l_1, l_2, \alpha) e^{-\alpha t} \quad \text{for } \alpha t \text{ large}$$

(1)

The first two properties have been observed in the 2D simulation of the model with the segment length $l_1$ and $l_2$ drawn with equal probability ($\alpha = 1/2$) [2]. In the same reference the difference in long-time behaviour between the case of equal probability mixing and the "pure case", $l_1 = l_2$ or $\alpha = 1$, has been noticed.

In order to check the validity of the previous properties, we have generalized this Monte Carlo simulation to various probabilities $\alpha$ in two and three dimensions.

We take lattices of size $L = 256$ and 512 in $D = 2$, and $L = 32$ and 64 in $D = 3$. The lengths of the deposited segments (in number of sites) range from $l = 2$ to $l = 12$ in 2D and 8 in 3D, so that, the ratio $l/L$ being small, we expect the finite size effects to be negligible. The time scale is fixed by setting $\delta t = 1/DL^D$ in order to allow a comparison with the exact 1D model of reference [3], where the time unit corresponds to the (averaged) time needed for reaching a given site with a given orientation. Actually to save computer time, the selected site is (randomly) chosen in the list of free sites and the corresponding time step is $\delta t/p_r(t)$ where $p_r(t) = (1 - \theta(t; l_1, l_2, \alpha))$ is the probability for a site to be unoccupied at time $t$. 

At each successful attempt the coverage is increased by the fraction $\frac{l_1}{L_D}$. On a finite lattice the jamming limit is exactly reached in a finite time which depends on the lattice size and which can be determined easily. For all the cases we have investigated, we found that this time of saturation is of order $t_s = 7/\alpha$ in our time units.

For each set of parameters $(\alpha, l_1, l_2)$, we perform from 50 to 200 independent experiments, and average $\theta(t; l_1, l_2, \alpha)$ over this sample. The fluctuations are small, allowing precise measurements.

We first fix our procedure by a comparison of a 1D simulation with the exact formula of reference [3], for the particular choice $l_1 = 2, l_2 = 4$ and $\alpha = 0.25, 0.50, 0.75, 1$. We set the lattice size to $L = 2^{16}$, large enough for the finite size and finite saturation time effects to be negligible. Actually, the jamming limit coverage, $\theta_\infty(l_1, l_2, \alpha)$ that we measure, coincides with the exact value up to four digits. Furthermore we have checked the time dependence by comparing the measured and exact values of:

$$r(t) = -\ln[\theta_\infty(l_1, l_2, \alpha) - \theta(t; l_1, l_2, \alpha)]$$

In figure 1, we have plotted this quantity as a function of $\tau = \alpha t$, for several values of $\alpha$. From the long-time behaviour of $\theta_\infty(l_1, l_2, \alpha)$ expressed in equation (1), we expect these curves to be parallel straight lines. The agreement between exact and measured values is total, confirming that the finite size effects are negligible. However, if we want to extract from these data the exponential long-time behaviour of equation (1), we find that for $2 \leq \tau \leq 5$ the slope of the straight line is slightly overestimated with respect to the exact asymptotic value, due to corrective terms in $e^{-2\alpha t}$. But for the simulation to give accurate results, the time $\tau$ must be less than the saturation time, which depends on the size of the lattice. Therefore, finite size effects occurs through the long time behaviour and precise determinations of the rate of the exponential decrease and of the prefactor, need large scale simulations.
Fig. 2. — The asymptotic coverage $\theta_\infty$ for the mixed case $l_1 = 4$ and $l_2 = 6$ as a function of the probability $\alpha$ of the shortest segment. $\alpha = 1$ corresponds to the pure case $l = l_1 = 4$ and $\alpha = 0$ to the pure case $l = l_2 = 6$.

Table I. — $\theta_\infty$ in 2D and 3D for different values of $l_1$, $l_2$ and $\alpha$, averaged over 50 independent histories on lattices of size $L = 256^2$ and $L = 32^3$. The typical statistical error is of some units on the last digit.

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Fig. 3. — The quantity $-\ln(\theta_\infty - \theta(t))$ as a function of $\alpha t$ resulting from our simulation in two (Fig. 3a) and three dimensions (Fig. 3b), for the case $l_1 = 4$, $l_2 = 6$ and the four values of $\alpha = 0.25, 0.50, 0.75, 1$, from the top curve ($\alpha = 0.25$) to the lowest one ($\alpha = 1$).

Turning now to 2D and 3D, we have measured $\theta_\infty(l_1, l_2, \alpha)$ for a set of values of the parameters $l_1$, $l_2$ and $\alpha$. The results are collected in table 1.

We may verify, using this data, all the properties of $\theta_\infty(l_1, l_2, \alpha)$ described above in 1D. Furthermore, we find that as $l_2 \gg l_1$, it quickly reaches a limiting value depending on $l_1$ and $\alpha$.

The discontinuous behaviour of $\theta_\infty(l_1, l_2, \alpha)$ as $\alpha \to 0$ appears clearly in figure 2, for $l_1 = 4$ and $l_2 = 6$ in the 2D case. When $\alpha$ decreases from 1, which corresponds to the pure case $l = 4$, to 0, $\theta_\infty$ increases towards a limiting value much larger than the $\alpha = 0$ one which corresponds to the pure case $l = 6$.

Another striking result concerns the time dependence of $\theta(t; l_1, l_2, \alpha)$. On the basis of the 1D results we expect it to be exponential in the variable $\tau = \alpha t$. In order to check this assumption we have plotted the quantity $r(t)$ defined in equation (2) as a function of $\tau$ for all the values of $\alpha$, $l_1$ and $l_2$ of the table I. Figure 3 displays the case $l_1 = 4$, $l_2 = 6$ for the four values of $\alpha$ in 2D (Fig. 3a) and 3D (Fig. 3b). It clearly appears that the curves are parallel, and linear for $\tau$ large enough. The slopes of all these curves range from 0.95 to 1.1, whereas the prefactor slowly depends on $\alpha$. As we have seen in the 1D case, an unbiased determination of the slope requires a high precision measurement. We have realised this experiment for the case $l_1 = 4$, $l_2 = 6$ on lattices of linear size $L = 512$ in 2D and $L = 64$ in 3D with 200 independent histories. We perform a linear fit of $r(t)$ (Eq. (2)) in an interval of $t$ which satisfies the following conditions (i) $t$ sufficiently large that corrective terms to the leading behaviour of equation (1) are small, and (ii) $t$ be less than the averaged saturation time in order to avoid finite size effects. The errors on the slopes are obtained by displacing this time window across the region $0.5t_s \leq t \leq 0.7t_s$ where $t_s$ is the saturation time. The results are $0.99 \pm 0.02$ in 2D and $1.00 \pm 0.02$ in 3D.

In conclusion, we have confirmed by a simulation that the salient features of the exactly solved 1D model of random sequentially deposited segments of different lengths are present in 2 and 3 dimensions. The trend for the asymptotic coverage to grow with the length of the largest segment, but to decrease with the length of the shortest one, is recovered. Furthermore, we check that the asymptotic coverage corresponding to only one segment length, discontinuously jumps to a larger value as soon as an infinitesimal mixture with shorter segments is allowed. If
the mixture is realised with larger segments, the coverage continuously grows as the proportion of large segments increases, a behaviour not so close to physical intuition as the previous ones. Finally, the exponential rate which dominates the long-time behaviour of the coverage, is shown to be exactly equal to the probability of drawing the shortest segment.

References