Surface Science 651 (2016) 182–186

Contents lists available at ScienceDirect

Surface Science

journal homepage: www.elsevier.com/locate/susc

Managing numerical errors in random sequential adsorption

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ARTICLE INFO

Article history:
Received 17 March 2016
Received in revised form 22 April 2016
Accepted 29 April 2016
Available online 03 May 2016

Keywords:
Random sequential adsorption
Saturated random packing
Errors in RSA simulation
RSA kinetics

ABSTRACT

Aim of this study is to examine the influence of a finite surface size and a finite simulation time on a packing fraction estimated using random sequential adsorption simulations. The goal of particular interest is providing hints on simulation setup to achieve desired level of accuracy. The analysis is based on properties of saturated random packing of disks on continuous and flat surfaces of different sizes.

1. Introduction

Unflagging interest in properties of random packings of different objects is a result of its application in description of soft and living matter [1,2]. One of the protocols that allows to create a specific type of random packing is random sequential adsorption (RSA). Such packings was used for the first time by Flory to study the attachment of blocking pendant groups on a linear polymer [3]. In 1960 Rényi studied the parking pattern of cars along an unmarked curb [4], which is another example of one-dimensional RSA. Its present popularity owes to Feder who has shown that it can be very useful for modelling monolayers obtained during irreversible adsorption processes [5–8]. Since then RSA algorithm and properties of random packings became an active area of research e.g. [9–11]. More recently, random packings generated by RSA have been in the range of interest of a number of other scientific fields, e.g., mathematics [12], telecommunication [13] and information theory [14].

The RSA algorithm is based on the following steps:

- a virtual particle's position (and orientation for anisotropic shapes) on a surface is drawn according to the specific probability distribution that reflects the structure of the surface. For example, the uniform probability distribution corresponds to a homogeneous surface.
- the virtual particle is tested whether it intersects with any of previously added particles. If not it is added to the packing. Otherwise it is removed and abandoned.

The steps should repeat until the packing is saturated, i.e., there is no room for any additional particle on the surface. The main problem of RSA is its efficiency at late stages of simulation, where a probability of adding subsequent particle is very small. Thus it requires then very large number of iterations and the method becomes ineffective. Therefore, a simulation is usually stopped after a large but finite number of iterations n and the number of particles in a saturated packing N is extrapolated according to the Feder's law [15–17].

$$N = N(t) + At^{-\frac{1}{d}}. \tag{1}$$

Here, $N(t)$ is a number of particles in a packing after dimensionless time $t = nS_p/S$, which measures number of iterations and is used to compare results of simulations using different sizes of a packing S and different sizes of a particle S_p. Parameter A is a positive constant and d is equal to 2 for disks and 3 for anisotropic shapes [18,19]. The relation is valid for large t. Such extrapolation is one of the sources of numerical error in designating N. Another one is a finite surface size S. Recently, Zhang et al. have proposed optimized version of RSA, in which sampling omits areas where there is not possible to place another particle [20]. This significantly speeds up simulations especially at the late stage of packing creation where most of the places are already occupied. This makes possible generating saturated packings of disks after a relatively short simulation time. In practice, however, this solution cannot be used for very large packings ($N_{\max}$ $_amp_$gt; 10^8) due to its memory requirements. Here, the memory is needed to store an information about places where sampling may result in adding a disk to a packing. Moreover, no extension of this method have been developed for anisotropic shapes, so far, thus, in general, an error resulting from

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http://dx.doi.org/10.1016/j.susc.2016.04.014
0039-6028/

extrapolation cannot be omitted. In the case of RSA, controlling errors is crucial when saturated packing properties are to be measured with high precision, for example to compare packing fraction for different but similar shapes [21].

The main aim of this study is to carefully analyse the influence of finite time of simulations and of finite size of a packing on the relative error of an average saturated packing fraction obtained in a numerical experiment based on RSA. Additionally, other properties of random sequential adsorption are examined, such as distribution of the number of particles in a packing as well as the time needed to saturate a packing. To achieve this, we studied saturated random packings and kinetics properties of RSA of disks for various surface sizes.

2. Simulation details

Surface area S varied between 10^4–$4\cdot10^7$, with a single disk area of $S_p=1$. Saturated packings were created on square surfaces of periodic boundary conditions, using method described in details in [20]. For each studied surface size, 100 independent packings were analysed with an exception of $S=10^6$, for which 10^4 packings were studied. For each disk in a packing, besides of its position, its sequential number and dimensionless time at the moment of placing it in the packing were recorded. Simulations were performed on a desktop PC with i5-4670K processor and 24 GB of RAM. The memory requirements depend mainly on accuracy of representation of a space where the next particle can be placed. More accurate approximation requires more memory but also may speed up simulation. Therefore, to perform simulations effectively a balance between memory consumption and computing time is needed. For example, for $S=10^6$ and using 1.7 GB of RAM or more, it was possible to create saturated packing in 75 s, but when memory consumption was limited to 1.4 GB of RAM only, the simulation time grows up to 730 s.

3. Results

The example of saturated packing of disks is shown in Fig. 1.

An important property of a random packing is its average packing fraction:

$$\theta=\left\langle N\frac{S_p}{S}\right\rangle, \tag{2}$$

where $\langle\cdot\rangle$ denotes averaging over a set of independent packings. The average is well defined and the packing fraction seems to be normally distributed (see Fig. 2). Although this observation seems to be trivial, note that the time needed to get a saturated packing behaves in a totally different way (see Fig. 3). Its distribution remains a power law, clipped for small values of t.

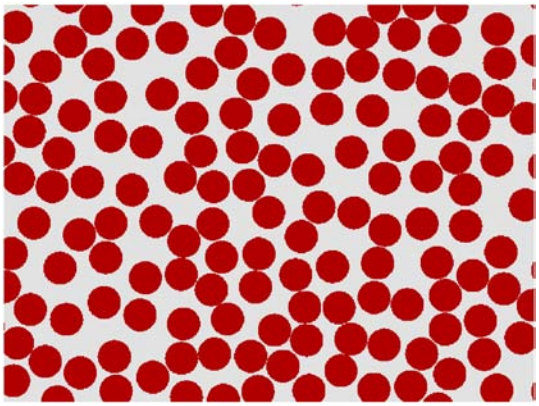

Fig. 1. Fragment of a saturated packing of disks obtained from RSA simulations.

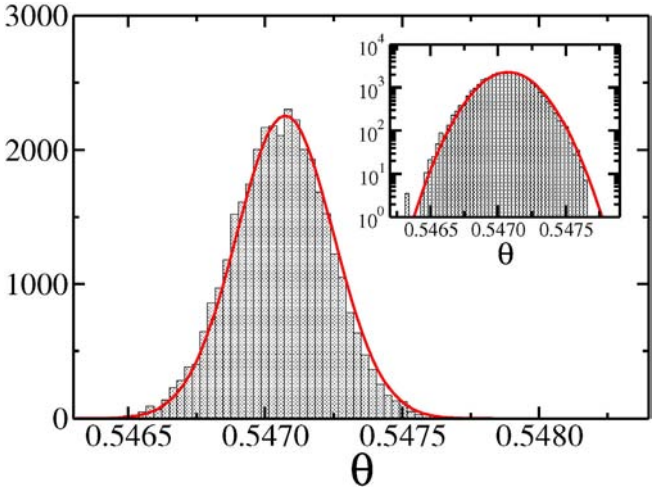

Fig. 2. Histogram of saturated packing fractions obtained from 10^4 independent packing for $S=10^6$. Red line corresponds to normal distribution of the average 0.547070 and standard deviation 1.76752×10^{-4}. Inset shows the same plot but in log-normal scale. Histogram was normalized to represent probability distribution. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

3.1. Dependence of numerical error on packing size

As this study focuses mainly on errors management, it is worth to analyse Fig. 4, which presents numerical results for an average saturated packing fraction for different packing sizes. This plot suggests that for quite large surfaces of periodic boundary conditions total error is practically equal to statistical error. Note, for example, the agreement between an average over 10^4 independent saturated packings for $S=10^6$ and average over 100 packings for $S=4\cdot10^7$. It is expected, as the intensity of finite size effects for periodic boundary conditions are strongly related to the correlation length over the linear system size. For one dimensional packing generated by RSA algorithm it was proved that density autocorrelations are super exponentially damped at long distances [22], and numerical experiments show that this damping is stronger when packing dimension increases [20,23]. Thus, for two dimensional case density autocorrelation function is practically equal 0 at a distance 10 times larger than the diameter of a disk.

Although some values in Fig. 4 are outside error bars limit, this also agrees with statistics. For a normally distributed variable, the probability

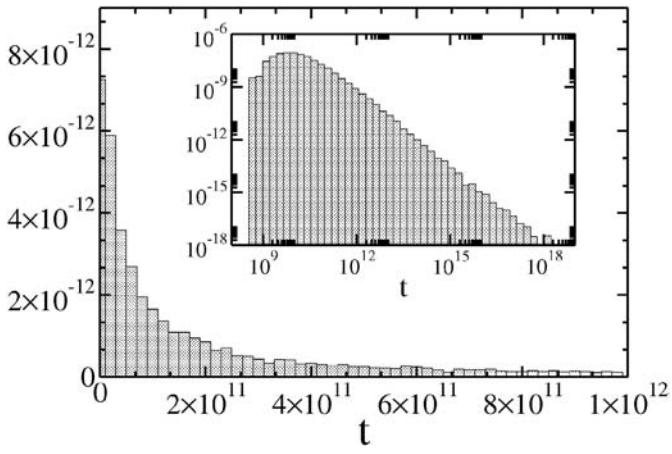

Fig. 3. Histogram of dimensionless time after which packing became saturated. Inset shows the histogram in a log–log scale. Note that in this case bins have different widths. Both histograms were normalized to represent a probability distribution.