# CONSTRAINED RANDOM WALK OF A CARRIER IN TWO-DIMENSIONAL SITE-PERCOLATION LATTICE, EXEMPLIFIED BY VIRTUAL AND REAL WORLD SCENARIOS\*

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A Random Walk (RW) realization in the square lattice, upon which a percolation cluster of sites, visited one by one by random walkers is built up (by direct Monte Carlo method), has been carried out towards its basic tendencies. It turns out that if the RW is realized near the site-percolation threshold, the process, as expected, decelerates. If, in turn, one systematically goes above the percolation threshold, being roughly about 0.6, towards the isotropic site-cluster regime, the process accelerates. Some drift superimposed on the RW realization as well as boundary conditions of certain types change the system behavior in a quite predictive way. Both new and interesting examples, emphasizing a possible applications of the phenomenon under study, are carefully mentioned. A finite-size effect always incorporated in the realized MC-algorithm is going to make the process apparently closer to reality. The notion of continuous phase (sub)transition has been discussed in the presented context.

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### 1. Introduction

Interest in disordered systems attracts nowadays constant attention of researchers and technologists. A huge variety of studies and examples devoted to the percolation problem enables to propose a statement that the problem is going to be one of the most important in modern statistical physics, and its "surroundings", like chemical physics materials science, biophysics, or soft-condensed matter theory, or even computer science.

The first class of theoretical challenges, inevitably associated with the subject of percolation, concerns with a question: Whether there are one or more infinite spanning clusters in the available physical space? The answer obtained just recently assures that there are, in general, more than one spanning clusters of infinite (or finite but very large) size [1]. This issue, however, will not be addressed in the present work.

The second class of fundamental theoretical questions is related to possible connections between very basic models of condensed-matter theory, like stochastic Ising or Potts models, Kardar–Parisi–Zhang systems, describing, for example, the dynamics of rough surfaces, and the percolation model. Some strict mappings of the systems mentioned on one another have been found in several cases [2]. But this will not be addressed in this issue, either.

Among many others quite specific sub-classes of problems, a fascinating class of theoretical tasks emerges, which is focused on the Random Walk (RW) problem in a disordered lattice of any reasonable kind [3]. This sort of problems will be a subject of the present study. Namely, in this work we are going to investigate the RW problem, realized by a direct Monte Carlo simulation on a square lattice, upon which a percolation cluster is built up. On this site-percolation cluster near and above the percolation threshold, RW realizations, one by one and by means of letting a "testing" particle (carrier) walk at random, have been carried out. After examining the socalled pure RW [4] on the percolation cluster close and a certain distance above the percolation threshold, that is known to be about 59 percent [5], we have superimposed certain constraints on its realizations, first enforcing the RW to be drifted, weakly, moderately as well quite strongly. Then, we have put into play other constraints, letting the system to feel its boundaries, mostly by presuming the elastic (weakly, moderately and strongly) as well as inelastic collision effects while touching the lattice border by the particle. Moreover, we put at least one heuristic solution<sup>1</sup>, which is also going to yield some type of small constraints while looking at the system behavior. Namely, it is made quite arbitrary to put the starting line to be the second

<sup>&</sup>lt;sup>1</sup> There are in fact a few more, which have, at the first stage of the performed computer simulation, been incorporated just for making the process a little bit more constrained *viz.* realistic, *cf.* Appendix for details.

column of the lattice. This is equivalent to push the walker in arbitrary way into right direction by one lattice  $constant^2$ .

Thus, the main purpose of this paper is to examine how do some physical constraints superimposed on the system influence its overall behavior. Another motivation to perform this computer-simulation-based work is to make the process under study as being realized under more realistic conditions, though the assumption of a testing multiparticle random walk (a 'multitask system') is unfortunately not perfectly fulfilled because of quite modest computational capacity being at authors' disposal. We hope, however, that a set of realistic examples chosen, and very much related to this study as well as some report on heuristics applied here, will somehow compensate the above drawback.

The principal quantity under vivid examination is the mean (first) passage time of a testing particle against the linear size of the available lattice space. Invoking the phase diagrammatic notion, let us stress that for dealing with a (dynamic) phase diagram some relation between the order and control parameters is undoubtedly needed. In the presented case, one can find such a relation while expecting some subtle relation between the probability of establishing the percolation phenomenon (density of the disordered flock) and some very dynamics of a RW realization in the site-percolation two-dimensional space, represented by the speed of an averaged RW, given as a ratio (in a logarithmic scale) of some two quantities, namely that going to represent linear lattice size as well as the passage time, being always a signature of meander-like features of the two-dimensional percolation substrate. Let us note here that by choosing the percolation probability either slightly or significantly above the percolation threshold, it is guaranteed, at least in statistical meaning of this word, that there is a connection between the left as well as right sides of the lattice, or that one of the disordered 2dmatrix main features appears to be its connectedness, so that a carrier's passage is expected to occur. As it is known, the main characteristics obtained classify the process to be not a normal RW, but a model phenomenon being quite sensitive to the above listed constraints, which, in turn, seems to be sometimes beyond a common-sense realization. (An impressive issue on this subject, considered formally, however, in a three-dimensional case, was also addressed under the term diffusion on a fractal during one of the preceding Smoluchowski Symposia, cf. Mazo in [6], and references therein.) We believe

<sup>&</sup>lt;sup>2</sup> To be precise, we have placed a carrier on an occupied spot in the second column, then we have pushed it, again arbitrary, by one lattice constant to the right (the experiment without drift), and then we let the carrier perform its random walk until it reaches an occupied spot in the last column; for obvious reasons, the experiment with drift did not include that arbitrary placement into the second column, but the start was always from the first column.

that something similar is going to happen in reality, what we are trying to exemplify by various physical contexts (scenarios), cf. [7] for having a look into a biophysical phenomenon. No doubt that examples can be found really everywhere, even unexpectedly, *e.g.* in the Internet traffic, where the information packets may "percolate" through a virtual space, which in terms of phase transition language means crudely that a certain passage between sparse (free) and versatile congested states of the complex system under investigation is going to occur [8].

# 2. Computer model, its outlines, peculiarities and basic signatures

The computer model, staying behind the presented study, is rather straightforward. Thus, we wish to explore the following algorithm:

- 1. Place arbitrarily a carrier in the second (without drift term) or first (with drift term) column of the lattice on a spot labelled by "1".
- 2. Let the carrier move at random (being drifted or not) on a percolation substrate composed of randomly distributed sites, denoted by "0" and "1", for empty and non-empty sites, respectively.
- 3. Look for the place into which the carrier is going to travel by one or more lattice units (constants)a) If it is a "0" spot, or a border site, repeat the sampling again, or apply some boundary rules, respectivelyb) If it is a "1" spot proceed further.
- 4. Update all counters, but after having assured, that the particle strikes the last lattice column at a "1" spot.
- 5. Go back to point 1 unless a stop command does intervene.
- 6. Complete the computation by carrying out some calculations and/or drawing pictures of interest.

As a result of thorough realization of the above algorithm, one may arrive at some numerical data, being gathered in the following two Tables. Let us, in short state what appears to be really remarkable while looking into the Tables, *cf.* Table I and II, respectively. It can be juxtaposed as follows:

(i) The phenomenon in question has been examined twofold: Either while some quite versatile boundary conditions (BCs) do influence the RW system, or, when (decisive) drifts of rather different types are going to be readily superimposed on the system behavior.

- (*ii*) Some small-scale computer simulation have been performed, where the lattice size ranged between  $2^3 \times 2^3$  and  $2^7 \times 2^7$ , *i.e.* over 5 binary "decades".
- (iii) The quantity of prior interest has been agreed to be the mean (first) passage time, that means, the number of steps that need to be realized just for traversing across 2d site-percolation structure from left (second column, cf. remarks in Sec. 1 and in Appendix, but a walker must begin its walk at a "1" spot) to right (last column, but a walker must strike it at a "1" spot). This quantity has been measured against the linear square lattice size, and averaged over 50 realizations for each lattice, cf. some details beneath, mostly involved in Tables I and II.
- (*iv*) Even under assumed constraints (see, point (i)) some well known basic tendencies of the RW temporal behavior have shown up [3, 4].
- (v) There exist certain interesting discrepancies when compared to a periodic boundary RW realization as well as while neglecting a drift, being assumed of quite different strengths. They are know from literature, *cf.* [3–5].
- (vi) There are some fairly expected items in the presented Tables, cf. captions to them, that can be quite well understood in terms of either very finiteness of the system under consideration and its realization(s) (first of all, realize that the values of the basic quantities obtained do depend upon the number of trials or realizations), or, while remembering that the studied system is classified to be pretty nonlinear viz. unpredictive, when one is going to change, even slightly, its constraints.
- (vii) A quite general scenario drawn, provokes someone to find out some suitable examples that may exemplify the temporal behavior of the model phenomenon under study; in our opinion, they can be somehow borrowed at least from two areas of research, namely from the virtual Internet world as well as from a quite real biophysical context, e.g. a diffusion of amphiphilic tracers in phospholipid monolayers [9]. In the former, one may think about passage of a certain information packet (a carrier) that successfully passes over many routers-influencing states, just to reach its destination place. In the latter, in turn, one can conceptually proceed in terms of a walk of some invasive spread that constantly affects its healthy surroundings, *i.e.* when it passes over its fitness landscape. Note, by the way that maybe the so-called smallworld model [10] would be more appropriate in this context, but one may realize that our model is (at least) formally immersed within this fashionable concept. Both these categories touch probably deeply the

notion of phase transition, possibly of the second order [11]. They both seem to have much in common at least with some two phase transitions, namely:

A. In the thin film formation, there appears readily to be a challenge how some experimentalist can manipulate between commensurability/incommensurability of a thin film deposited (sputtered) on the substrate of a certain crystallographic characteristics; here, a suitable collective dynamics, making use of some structural but dynamic correspondence between the deposit and the (solid) support must be the case, *cf.* the Frenkel–Kontorova model of thin film formation, which, in terms of thermodynamic phase transition behavior leads typically to a phase diagram à la some degree of commensurability (order parameter, frequently measured in percents) as a function of an external parameter, *e.g.* a lateral pressure;

B. In collective traffic behavior under periodic boundary conditions, however, one observes a motion of individuals under versatile noise strength conditions, leading to self-propelled behavior; it leads to a certain ferromagnetic vs paramagnetic-like phase transition behavior, or more generelly that being of order/disorder type [12]: Note, however that the latter cannot be confused with phase transition of second order, though there are some (unresolved) relations between them, cf. the Bose–Einstein condensation as a landmark case [11, 13]. (Notice that we did not explicitly examine the influence of fluctuations on the system behavior. This probably remains to be a quite interesting future task.)

From Table I it can be seen that the RW behavior has been examined in three subgroups. In the first subgroup (first 4 rows) we anticipate, within the simulation accuracy, some usual RW behavior being only slightly influenced by the boundary constraints, which are assumed to be the simplest reflection BCs. When some increase of elastic response of the boundary to the carrier is playing a role (second subgroup, equivalent to the three next rows in the table), the limit  $\frac{1}{2}$  is approached more visibly, and all the exponents are augmented, when compared to the previous ones. In the last subgroup, where some inelastic BCs [15] have been applied, one detects possibly smallest scatter of the exponent values, since the two-dimensional RW is sometimes, *i.e.* along the boundaries, realized as the one-dimensional one.

In Table II, in turn, one recognizes some influence of various drift terms. A general conclusion towards a system tendency can be risked, namely: The bigger the applied drift is, the more pronounced is the system tendency just to approaching the exponent value of 1, *i.e.* to reach a "first" noticable limit characteristic of the so-called supernormal RW, *cf.* discussion in the next

#### TABLE I

Statistics obtained from the performed direct *Monte Carlo* computer simulation, cf. [14], for the so-called <u>undirected</u> (pure) RW process, with simplest reflecting and more specific non-weakly reflecting as well as non-reflecting boundary conditions, respectively, cf. Appendix. They are abbreviated by el0, el1 and iel, respectively. The average confidence level of the presented results is ca. 99.4 percent, which may for sure be affected by both the heuristics invented for the simulation purpose as well as the finite size effect, due to not too large linear size of the square lattice (the maximum value is assumed to be 128 lattice units, cf. text for other details), which generally emphasizes quite nonlinear behavior of the averaged single-particle traffic [15]. Notice that the value of  $d_w$  in the 4-th row appears to be somewhat bigger than it is reported, *i.e.* about 0.491, and slowly but surely reflects a tendency to reaching  $\frac{1}{2}$ .

$\operatorname{Exponent}(\widetilde{d_w})$	Probability $(p_{per})$	$\operatorname{Drift}^*$	BCs**
0.34	0.60	0	el0
0.46	0.80	0	el0
0.49	0.98	0	el0
0.49	1.00	0	el0
0.35	0.60	0	el1
0.52	0.80	0	el1
0.50	0.98	0	el1
0.39	0.60	0	$i \mathrm{el}$
0.48	0.80	0	$i \mathrm{el}$
0.49	0.98	0	$i \mathrm{el}$

\* Zero drift has been applied.

\*\* In the first 4 rows some possibly simplest reflecting BCs have been applied (return by one lattice unit after reflection). In the second 3 rows a bigger variable reflection of the carrier must be anticipated (see, Text), while in the 3 last remaining rows some inelastic collision, leading to a one-dimensional random motion of the carrier along the boundary, has been introduced.

Section. The lowest limit with  $p_{per}$  appears to be interesting since it is going to fix the value of the  $\tilde{d}_w$  exponent around 0.27–0.28 for any pronounced drift value, *cf.* Appendix for details.

Note also, which is characteristic of both the tables under analysis, that some other relation has to be mentioned. Namely, if one goes away from the percolation threshold, being about 0.6, towards the isotropic phase, with probability equal to 1.0, one sees that the distance in the probability space has increased about  $\frac{2}{3}$  of the threshold probability mentioned, whereas the

Statistics obtained from the performed direct *Monte Carlo* computer simulation, for the so-called <u>directed</u> RW process, with simple (possibly weakly) reflecting boundary conditions (BCs), but for various types of drifts, superimosed on the RW behavior. The average confidence level of the presented results is about 97.8 percent, *cf.* remarks in Table I, and consult [15] for some details. The values in rows from 5 to 7 appear to be a bit surprizing, especially while compared to those in the first 4 rows, which would probably draw a certain attention to both the limits (some need to continue the simulation task emerges) as well as 'nonlinearities' of the performed computer experiment.

Exponent $(\tilde{d_w})$	Probability $(p_{per})$	Drift●	BCs●●
0.28	0.60	Max	el0
0.70	0.80	Max	el0
0.90	0.98	Max	el0
0.92	1.00	Max	el0
0.28	0.60	$\max$	el0
0.85	0.80	$\max$	el0
1.00	0.98	$\max$	el0
0.27	0.60	$\operatorname{mid}$	el0
0.77	0.80	$\operatorname{mid}$	el0
1.00	0.98	$\operatorname{mid}$	el0
0.31	0.60	$\min$	el0
0.73	0.80	$\min$	el0
0.78	0.98	$\min$	el0

• Possibly biggest (Max), somewhat smaller but also big (max), some intermediate (mid) as well as possibly smallest (min) drifts have been used, respectively, *cf.* explanations in Text as well as the Appendix.

•• The boundary condition is always the same, *i.e.* the simplest elastic one, denoted as in Table I by el0.

exponents have experienced some "outgrowth" from ca.  $\frac{1}{3}$  (more or less) up to  $\frac{1}{2}$  ('normal case'), or even up to 1 ('supernormal case'), *i.e.* they increased by  $\frac{3}{2}$  or even by 4 times (drift<sup>•</sup>), respectively, *cf.* Appendix. It resembles at first look some colonization or infection scenario by a soil-borne fungal plant parasite, exhaustively explored in [7], and interpreted quantitatively in [10]. It will be commented in detail in one of the subsequent sections.

It is worth to mention some theoretical realizations of the routes that must be passed more or less collectively (or, one by one but under a set of realistic constraints, as is done in this work). One may recommend here at least two types of descriptions. The first one, being the most popular, is based on the Einstein's concept of the mean-squared displacement (appreciated also by Smoluchowski [16]), and can be summarized by the following formula [3,5]

$$\langle r^2(t) \rangle \sim t^{2/d_w} \,, \tag{1}$$

where the left-hand side expression denotes the above mentioned key quantity, being proportional to the area, or a number of sites, visited by a walker (t is the time, and  $d_w$  stands for a RW dimension), whereas the second is provided by a discretized master equation of Smoluchowski-like type, given by [17,18]

$$\frac{d}{dt}n_i(t) = -\Sigma_j W_{ij}n_i(t) + \Sigma_j W_{ji}n_j(t), \qquad (2)$$

for which site-probabilites  $n_i$  as well as transition rates  $W_{ij}$  (and  $W_{ji}$ ) are some quantities of prior importance.

Especially the W probabilities applied particularly for traffic phenomena, are strongly suggested to be chosen in a form [19]

$$W = \frac{\Phi}{\tau},\tag{3}$$

where  $\Phi$  stands for a prefactor, enabling one to include proper optimization conditions for the analyzed traffic conditions (in case of  $W \equiv W_{ji}$ , one provides  $\Phi = 1$ , but in the countercase  $\Phi$  is a combination of  $W_{ij}$ 's), whereas the parameter  $\tau$  is a time constant, which can be understood as the waiting time for the escape of a carrier out of a jam or some congestion state into unperturbed (free) flow. Look also into [12], pp. 377–382, where a phase transition scenario, like free vs synchronized (correlated) flow as well as its relations to a jam state have been drawn, cf. Fig. 1.

Note, by the way that in Fig. 1 the plotted curves represent the congested dynamic phases ("ferromagnetic phases"), cf. [20], where the applied drift ("ordering external magnetic field") makes the information flow more pronounced, enabling to reach values above 180, *i.e.*  $\tilde{d}_w \to 1$ , cf. Table II. It is then a kind of differentiation between unproperly ( $\tilde{d}_w \to \frac{1}{2}$ ) as well as properly ( $\tilde{d}_w \to 1$ ) congested phases. If uncertaintity level tends to zero, the phases become to be non-congested, but a really free ('absolutely non-jamming') [8] phase appears above the abscissa ("paramagnetic phase"), for which such a simple statistical measure of information uncertainty, invented *ad hoc* for the congested phases, does not hold (because it is not deterministic!), or can, *e.g.* artificially, be completed by adding new points on the ordinate, the values of which exceed 100 in this case (obviously, the spontanous "magnetization" would disappear). Information Uncertainty



Schematic figure, representing some information diagram of the second Fig. 1. order type (continuous) [11], in which the so-called information uncertainty stands for a control parameter ("temperature") while the (dynamic) order parameter is chosen to be the information flow. The former is evaluated to be  $-k \times \ln (p_{per})$ , whereas the latter stands for the ratio  $\frac{\ln (L_{sql})}{\ln (T_{mfp})}$ , but also multiplied by k, which is just  $k \times \tilde{d_w}$  ("dynamic magnetization"), cf. Tables I and II; here  $L_{sql}$  represents the linear lattice size, whereas  $T_{\rm mfp}$  is the mean first passage time (the arithmetic mean was always taken over 50 simulation runs for each  $L_{sol}$ , ranging from 8 to 128), and k stands for some adjustment ("Boltzmann") constant, k = 200. The k constant is chosen roughly to give the ranges of both ordinate and abscissa axes of the diagram not exceeding 100 (percents), but for the set of data from the Table I (first four rows, cf. the steepest curve). The diagram is based on the first four rows taken from Table I (zero drift, the left steeper curve) as well as Table II (nonzero drift, the right more "extended" curve), so that it is not a smooth curve, but reflects rather main tendency of the stochastic process under study, with some crossover towards lower values, cf. Text as well as [23]. Notice that for the both cases (curves) presented the same boundary conditions, denoted by el0, cf. captions to Tables, have been assumed.

The present authors would propose to consider some phenomenological extension of Eq. (3), just in the form of  $W = \frac{\Phi}{\tau^{\mu}}$ , where  $\mu$  provides some necessary information of the RW ("network") topology, quite in a spirit of some well-known dispersion parameter h, closely related to the so-called spectral dimension [3,4], e.g. for  $\mu = 0$  ("free" motion) one gets a completely random route for a hopping carrier, but for  $0 < \mu < 1$  one detects a correlated, or even some highly correlated *viz.* jammed, movement, *i.e.* when  $\mu \to 1$ . A question arises: Whether such an extension proposed could be equivalent to a fractional order [21] master equation

$$\frac{d^{\mu}}{dt^{\tilde{\mu}}}n_i(t) = -\Sigma_j W_{ij}n_i(t) + \Sigma_j W_{ji}n_j(t) , \qquad (4)$$

where the time derivative  $\frac{d}{dt}$  from Eq. (2) has to be replaced by a fractional order derivative  $\frac{d\tilde{\mu}}{dt^{\mu}}$ , and  $0 < \tilde{\mu} < 1$ , since the sensitivity of the transport phenomena in question to the time scale, *cf.* [16], and refs. therein, appear to be quite noticable, and whether  $\mu \simeq \tilde{\mu}$  or not, or how they are mutually related, if this is the case? Moreover, maybe there exists a certain mutual relation between the exponent  $\tilde{\mu}$  and the RW exponent  $\tilde{d}_w$ , the values of which one can find in Tables I (no drift) as well as 2 (with a drift)? Some statistical-physical arguments, based on the Liouville kinetic equation [11] and concerning the so-called nonequilibrium phase transformations suggest [22] that

$$\tilde{\mu} \approx 2d_w \,, \tag{5}$$

so as a standard RW temporal behavior, *cf.* Table I, could be recovered, if one assumed  $\tilde{d}_w = \frac{1}{2}$ , which is equivalent to  $\tilde{\mu} = 1$ , *i.e.* when the ordinary time derivative comes into play, *cf.* Eq. (2).

Notice, however that both the main mechanisms mentioned above lead unequivocally to ending up with the asymptotic formula like Eq. (1), or its analytical, *i.e.* transformed, equivalents, *cf.*, so as a scaling behavior could quite often be recovered. A main shortage of such analytical descriptions, however, is that they are not capable of including such importants 'details' (read: constraints), like those studied here. That is why we try to invent or simply use the computer models. (A main advantage is, however that they are more under control, though up to a certain limit, sometimes named the approximation.) For a review of recent works on the diffusion on a percolation cluster, but applied specifically to chemical reactions involving proteins, one is encouraged to see [18], where the distribution of the mean first passage times as well as some analytical formulae of how to get them, having known that distribution, have been provided.

#### 3. Example(s) coming from the physics of Internet

In the doctoral dissertation by Kensuke Fukuda, a study of phase transition phenomena in Internet traffic has been presented [20]. Among many quite interesting details, ranging from statistical physics to computer science, one may experience some quantitative impression about the probability density as well as corresponding peak position of the flow density (packets' density) at a Japanese gateway, called the WAN Keyo, the abbreviation of the Wide Area Network at the Keyo University in Japan. The plots presented there show a dynamical phase transition behavior, where a transition takes place between congested as well as non-congested information flow phases. In the phase transition the order parameter has been chosen to be a peak position (in kbyte/sec) for some information packet (but averaged), occuring with a certain probability. The control paramter, in turn, has been correspondingly selected to be the mean flow density, measured in kbyte/sec, too.

In fact, a few transitions have been revealed, in particular between noncongested (free) and moderately congested flows. There appears to be a (weak) transition between moderately congested as well as heavily congested flowing phases, which can probably be better termed a crossover behavior [23], taking place within the entire dynamic phase, being called the congested phase; one could also argue that a subtransition is expected to occur, cf. [21]. The general phase transition diagram, which can be drawn, looks solely like the second order phase transition picture, cf. [20], and Fig. 3.7 therein.

We are of the opinion that our RW study on the percolation substrate can also reveal the behavior of such a type, though we may have certain problems of how to approach the Internet reality, *i.e.* how to get from our model some desired, eg. temporal characteristics, like *congestion length* distributions [24], round-trip times distributions [25], or even login-logout interval time distributions [26]. We mean that a first step towards the Internet specifics could be to support each randomly hopping carrier by a kind of protocol that has to contain: Some necessary information about its destination place, number of trips across the lattice (we have realized here one trip from left to right of the lattice), waiting, or temporary trapping times (whatever it means), and their distributions [27], strength of the drift superimposed on the walk as well as how does it may feel the boundary conditions ("geometric" limitations of the walk or cut-offs). We have actually taken into account the two last items mentioned, and some extention of the computer model could be towards incorporationg the three remaining ones. Moreover, we can also, even in such a simple computer experiment, introduce a notion of the *self-learning* RW that will take some advantage from what the preceding one has actually experienced while randomly traversing the matrix [28]. *i.e.* for how long as well as possibly where certain trapping events took place. (In the small-word language [29], it could be transferred to a change as well as some placement variation of local interactions of the carrier with its environment<sup>3</sup>.) In consequence, it can cause the protocol to be updated, so that a kind of RW with memory may be used as a straightforward generalization of this simulation scheme. It can, but in a continuous time domain, be supported by using the concept of the fractional Kramers equation (with a drift term), called the fractional Fokker–Planck equation, but with special emphasis put on its Rayleigh limiting case (with no drift term), derived for a test particle of mass M performing its Brownian motion via colliding with bath particles of mass m, where  $\frac{m}{M} \ll 1$ , which results in having collisions

<sup>&</sup>lt;sup>3</sup> In fact, the nature of the applied constraints can be a controlling factor for some qualitative differentiation among certain classes of random sets.

as being frequent, but not too weak, cf. [30], so that a kind of Levy flight might still be observed. In that case, by the way, the fractionality, involved by means of the Liouville–Riemann integral operator, concerns with the position space [30], but not with the time domain, as was discussed above. Last but not least, we have probably to revisit the meaning of the lattice, mostly towards Internet topology [31]. Also, the type of percolation, whether there must be the site- or bond-percolation [32], or mixed, or maybe coloured [33], *etc.* should be decided prior to a concrete experiment. At this stage of our presentation, we may say that, at least qualitatively, our model conforms well to that invented by the Japanese authors [8,20,26]. Moreover, we have practically estimated the main *length vs time* characteristics, which according to Tables I and II, appear to be power laws similar to that mentioned in Eq. (1), namely

$$L_{\rm sql}^2 \sim T_{\rm mfp}^{\ \varepsilon},$$
 (6)

where  $\varepsilon = 2\tilde{d_w} cf$ . captions to Tables I and II as well as Fig. 1 for details. Under the constraints applied, it is then a manifestation of (statistical) selfsimilarity, which stands for another landmark feature of the studies realized by the authors [20,25,26], but is also stressed in some other work [31]. By the way, notice that the RW is expected to be subnormal, when  $\tilde{d_w}$  is going to be less than  $\frac{1}{2}$  (or,  $\varepsilon < 1$ ) [3]. If, in turn,  $\tilde{d_w} > \frac{1}{2}$  (or,  $\varepsilon > 1$ ) the RW is said to be supernormal (*viz.*, "turbulent") [27,34]. The "singular" point  $\tilde{d_w} = \frac{1}{2}$  (or,  $\varepsilon = 1$ ) yields the so-called normal, *i.e.* Brownian behavior, *cf.* [13]. Note that the left-hand side of Eq. (6) gives straightforwardly the area of the lattice, though the overall area, due to heuristics presumed, *cf.* Sec. 2 and 5, is unfortuantely not used in full for the drift-free case, what would cause a systematic but negligible error for smaller lattices as well as for short-times RW realizations, see Appendix again.

### 4. Example(s) coming from the physics of natural habits

Similar scenarios like that presented in the preceding section can for sure be found *e.g.* in biophysics, or in even more specialized natural sciences. For instance, in colonized (saprotrophic) as well as parasitic pathogen fungal systems in soil activities occur practically in two-dimensional spaces that means, in soil layers [35]. In such systems, there appears naturally a certain contact distance necessary to undertake the spread of the colony. This distance would *a priori* correspond to the threshold probability of the percolation matrix (a support comprised of agar as well as nutrient spots, *etc.*), on which the epidemy is going to spread out. Such a situation was extensively analyzed in [7] in terms of basic percolation characteristics for a special type of fungal plant pathogen named *Rhizoctonia solani*. The results clearly show that above a certain critical distance between hosts at most a finite spread is observed while below that distance one may encounter an appreciable spread of the disease.

There are, however, some signatures of more subtle behavior in the (theoretically) unlimited growth regime, *i.e.* above the percolation threshold,  $p_{\rm cr}$ that can be anticipated by inspecting Fig. 1b (right in the middle) in [7], which above the percolation threshold is qualitatively of the same type like Fig. 1 in our study. (For obvious reasons they are, however, smoother.) The situation in which the colonization distance changes from smaller (large invasion) to bigger (small or even small and localized invasion) would correspond to a systematic change of the drift, from the largest to the smallest, cf. Table II, and analysis thereafter. In fact, one can even propose to compare the donor-recipient distance for such (small-world) systems [10], designated by  $d_{\rm cr}$ , and relate it to a maximum (average) time in which a certain number of sites has been colonized  $(T_{col})$  (provided that the process behaves further in a more or less stationary mode), just by making, correspondingly to  $\tilde{d}_w$ from Table II or I, a logarithmic ratio like  $\frac{\ln (d_{cr})}{\ln (T_{col})}$ , that means, by arranging a flow measure this way. It must then be plotted against a relative distance taken from the smallest  $d_{\rm cr}$ -values, say  $\dot{P} = (d_{\rm cr} \overset{i-{\rm th}}{-} - d_{\rm cr} ^{\rm min})/d_{\rm cr} \overset{\rm min}{-}, cf.$ Fig. 7 in [7], and also taken in a logarithmic scale as  $-K \times \ln(P)$ , where K could be some accomodation prefactor, cf. Fig. 1 (for assuring proper depiction such a prefactor should also complete the logarithmic ratio representing the invasion flow, whereas  $-K \times \ln{(P)}$  is likely to represent the invasion uncertainty or decolonization strength, according to a "schedule" given in the caption to Fig. 1, and description provided in Text).

Unfortunately, such a suggestive comparison, like that (a priori) proposed above, yields some exponential decay, which confirmes that presented in Fig. 8a in [7], so that this cannot readily correspond to what we present in Fig. 1. Some other well-behaved measures of the process are to be proposed to reflect that kind of behavior as pictured in Fig. 1. We have probed the following reasoning. Instead of P given above, we propose to use the colonization probability 1-P, and its natural logarithm, and for a flow measure we just choose  $\frac{\ln(N)}{\ln(T_{\text{resc}})}$ , where N represents the number of sites colonized, and the time  $T_{\text{resc}}$  is a (rescaled) colonization time (all the data are taken from Fig. 2). The rescaled time  $T_{\text{resc}}$  reads

$$T_{\rm resc} = T_{\rm ref} \frac{\Delta N}{N}, \qquad (7)$$

where  $T_{\text{ref}}$  is equal to 28 days, *cf.* Figs 7 and 8 in [7], and  $\frac{\Delta N}{N}$  is a relative change in the consecutive numbers of colonized sites. If we choose properly magnification factor(s), we are able to get satysfying, at least qualitative agreement with plots presented in Fig. 1; here, we have found a parabolic fit.

Let us also state explicitly that on the basis of our simulation, a tacid working assumption can be made, which states that there is, according to some quite visible correlations present in Table II between the drift strength as well as the values of  $\tilde{d}_w$ , taken for different percolation probability, a correspondence between the drift magnitudes, *cf.* Appendix, as well as the probability values. It was also used for inventing a comparison between our study and that published in [7]. This is as well a proposition on how our model can be transferred into an invasive percolation process [36, 37], and how both the models analyzed belong to a class of small-world models [10,29], where some meaning of the critical distance seems to be of crucial importance.

To finish the comparison, let us state that in contrast to our model the data presented in Fig. 7 in [7] are provided for the triangular lattice, for which  $p_{\rm cr} \approx 0.35$  [3,33]. To sum up, both the phenomena compared undergo roughly a scenario called the invasive spread (for replicate microcosms), depicted for different times after innoculation, *cf.* Fig. 4 (left column with pictures) in [7]. This kind of spread can indeed be chosen as a representative scenario, conforming well to our computer model, though in our model we do recognize somewhat different schedule, since the invasion occurs stepwise, because particles are launched one by one from the right-hand side of the lattice.

## 5. Concluding address

- The RW has been named a constrained random walk [38], because two types of constraints<sup>4</sup> have been superimposed in a systematic way on its behavior. They are subjected to either the boundary conditions, *cf.* Table I, or they arise as a result of trying to make the walk directional. Clearly, some tendencies of the discrete stochastic dynamics [39] in question have been picked up, and no definitely ultimate but rather fairly decisive conclusions can be offered.
- We wish to state that the process of passing the 2d percolation marix by the 'averaged' walker (a carrier or messenger) experiences (at least) a crossover from a normal to subnormal (*i.e.*, towards lower exponent values) or supernormal (that means: towards higher exponent values), according to the constraints proposed in the paper.

<sup>&</sup>lt;sup>4</sup> Referring to G.H. Weiss understanding of constraints that are either due to boundaries (exactly the case studied in the present paper) or they are subjected to keeping some characteristic quantity fixed, *e.g.* the end-to-end distance in statistical mechanics of polymers; the notion of constraints, according to Weiss, does not involve any possibility of taking a drift as one of the constraints, but the author readily differentiates between unbiased (undrifted) as well as biased, *viz.* directional RW. It makes some subtle but marked difference between our practical realization and what in [38] was ment.

- There is, however, something more interesting viz. more applicable in the process studied: An evidence of appearence of the transition of second type [11] appears, and a (dynamic) diagram of the sort free vs congested traffic, or comparatively, commensurate vs incommensurate adsorption effect in thin films' systems (a model system: Kr on graphite) can certainly be drawn [40].
- Heuristics as well as other factors of "secondary importance" (e.g., a certain asymmetry of the square lattice used, cf. the two first sections, which would imply that in some cases we have, in fact, used a "rectangular" lattice for which one side differed practically from the other by one latice unit) modify slightly the presented results, but do not destroy the main tendencies, cf. Appendix below.
- One is able to juxtapose a set of examples which stays behind the modeling proposed, *cf.* Sections 3–4. Moreover, one is capable of extending the list of examples by invoking at least a few more. It can even be done without referring to the seminal literature of the subject matter [1,3,4,33,38], but can be accomplished, *e.g.* by mentioning some practical realizations within the field of physics of (bio)materials, devoted either to a gas-fraction permeation study through porous polymeric membranes or to some defect formation process in model lipid materials, respectively, *cf.* [41]. A power-law behavior as well as time dependency of some basic kinetic coefficients [42] seem to be often manifested in those complex systems, *e.g.* networks in soil physics [43], where some interaction of randomly travelling particles with a disordered lattice appears to be a key feature.

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# Appendix

#### Some quantitative comment on the heuristics applied in the RW realization

As was announced before, the RW has been realized for a few different sizes of the square lattice  $L_{sql} \times L_{sql}$ , where  $L_{sql} = 8$ ; 16; 24; 32; 48; 64; 96; 128, but for different boundary conditions (elastic and inelastic reflection BCs), without a drift as well as for four different drifts, denoted by Max, max, mid, min, from the biggest to the smallest, respectively.

In all the cases without drift we are obliged to take into consideration initial condition (IC), *cf.* the first point of the algorithm in Sec. 2.

In the computer experiment without a drift (Table I) the IC is necessary. It is introduced to shorten the computer simulation, because this way we get rid of every first back steps (probability that the first step will be to back direction is  $\frac{1}{4}$ , but after this step we may loose the carrier, which will cause to start walking with a new carrier). Thus, this IC makes the real space available for travelling not a square space but that of a rectangle of size  $L_{sql} \times (L_{sql} - 1)$ . Such a modification would fortunately cause minor differences<sup>5</sup> while evaluating the exponent  $\tilde{d}_w$ , which can be recast based on the ratio

$$\tilde{d_w} \simeq \frac{\ln [L_{\rm sql}(L_{\rm sql} - 1)]^{1/2}}{\ln (T_{\rm mfp})}.$$
(8)

When instead of the geometrical mean in the logarithm's argument in Eq. (8) either the corresponding arithmetic or harmonic means have been applied, the value of the exponent becomes unchanged within assumed accuracy level.

For the case with a nonzero drift (Table II) the real size of square lattice is still  $L_{sql} \times L_{sql}$ , because the carrier is readily drifted from an occupied spot in the first column of the lattice, in which it is located.

The BCs applied, *cf.* Table I, mostly imply a certain reflection from upper and lower parts of the border of the lattice. For the elastic reflection a maximum reflection,  $d_{\text{ref}}$ , is an integer part of  $2 \times (1 + \frac{L_{\text{sql}}}{10})$ , and it describes how long could be a back step after a reflection from the border, measured in lattice constants, can be experienced by a walker. The values of  $d_{\text{ref}} \equiv d_{\text{ref}}(L_{\text{sql}})$  are 3, 5, 6, 8, 11, 14, 21, 27, and correspond to the values of  $L_{\text{sql}}$  listed above.

We see that the quantity  $d_{ref}(L_{sql})$  is a linear function of  $L_{sql}$ . We can quantitatively describe this relationship by proposing a simple linear fit

$$d_{\rm ref}(L_{\rm sql}) = A + BL_{\rm sql} \,, \tag{9}$$

where A = 1.4648 and B = 0.2002. Even such a specific though linear (it is important!) choice ensures a kind of regular reaction from the border while increasing the linear lattice size [15]. It looks also that our RW system is going to be stable against a linear (boundary-influenced) perturbation.

As was stated before, in our computer experiment we have used four types of drifts: Max, max, mid and min. The values of this drifts are:  $Max = L_{sql} - 2$ ,  $max = L_{sql} - 4$ ,  $mid = (L_{sql} - 2)/2$  and min = 2 [15]. These

<sup>&</sup>lt;sup>5</sup> E.g., while evaluating the exponents near the percolation threshold for  $p_{per} = 0.6$ , the obtained values are increased by ca. 0.01 when compared to those gathered in Table I.

are, however, some assumed values, because in practice after performing a drifted shift, the particle could land on an empty place, so that it must be shifted back along the longitudinal direction until a non-empty place has successfully been met. Looking at the values in Table II, we may state that the magnitude of the drift makes no essential difference when chosen appreciably large, at least near the percolation threshold as well as isotropic lattice limits. At some intermediate values one may expect some differences. While being chosen "unproperly", however (last three rows of Table II), the measure of information flow manifests a certain abnormal behavior, and would tend to behave as in the undrifted case near the percolation threshold, but then quite unexpectedly, rather. This can be explained as a separate type of temporal behavior in the disordered structure under study.

Moreover, one should note that if we change  $p_{\text{per}}$  in range between 0.6 and 1, *i.e.* we do observe some increase of  $p_{\text{per}}$  in value by  $\frac{2}{3}$  (still the drifted case is considered), but in the same time, one has to observe strong growth of the exponent  $\tilde{d}_w$  from 0.28 to 1, *i.e.* by about factor 4. However for the undrifted case and for the same increase in  $p_{\text{per}}$ , one experiences a growth of the expenent by factor  $\frac{3}{2}$ , which means ca. three times slower than in the drifted case, see Table I and Table II.

For those who may have some opportunity to go over [15] a more traditional way of studying such problems can be envisaged [44]. It has to be done by defining a (time-lag influenced) diffusion coefficient  $D = \frac{L_{sql}^2}{4T_{mfp}}$ , and thereafter, by checking its basic tendencies while using data available in seven tables presented in [15]. The cross-checking proposed aggres well with what was revealed in our study, *cf.* Sections 2 and 3.

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