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First-passage times in complex scale-invariant media

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How long does it take a random walker to reach a given target point? This quantity, known as a first-passage time (FPT), has led to a growing number of theoretical investigations over the past decade[1]. The importance of FPTs originates from the crucial role played by first encounter properties in various real situations, including transport in disordered media[2,3], neuron firing dynamics[4], spreading of diseases[5] or target search processes[6–9]. Most methods of determining FPT properties in confining domains have been limited to effectively one-dimensional geometries, or to higher spatial dimensions only in homogeneous media[1]. Here we develop a general theory that allows accurate evaluation of the mean FPT in complex media. Our analytical approach provides a universal scaling dependence of the mean FPT on both the volume of the confining domain and the source–target distance. The analysis is applicable to a broad range of stochastic processes characterized by length-scale-invariant properties. Our theoretical predictions are confirmed by numerical simulations for several representative models of disordered media[10], fractals[3], anomalous diffusion[11] and scale-free networks[12].

Transport properties are often characterized by the exit time from a sphere t_{exit}, which is the first time a random walker reaches any point at a distance r from its starting point. This quantity is well known for brownian motion in euclidean spaces, and has also been evaluated for finitely ramified deterministic fractals[13,14]. In these cases, the length-scale-invariant properties of the walker's trajectories have a key role and lead to the scaling form $t_{\mathrm{exit}} \propto r^{d_{\mathrm{w}}}$, which defines the walk dimension[3] d_{w}. Interestingly, it has been shown that a large class of complex scale-free networks are also invariant under the length scale renormalization scheme defined in ref. 15, even if they are of 'small world' type—that is, if their diameter scales like the logarithm of the volume. This remarkable property led the authors of ref. 12 in particular to characterize the mean exit time in this class of small-world networks by a set of scaling exponents.

However, in many situations, the determining quantity is not t_{exit}, but rather the FPT of a random walk starting from a source point S to a given target point T. Indeed the FPT is a key quantity to quantify the kinetics of transport-limited reactions[14,16], which encompass not only chemical or biochemical reactions[17,18], but also (at larger scales) interactions involving more complex organisms, such as a virus infecting a cell[19] or animals searching for food[6]. The relevance of the FPT has also been recently highlighted in ref. 12 in the context of scale-free networks, such as social networks[20], protein interaction networks[21] or metabolic networks[22]. The FPT and the exit time in fact possess very different properties. Indeed, the exit time is not sensitive to the confinement, as only a sphere of radius r is explored by the random walker. On the contrary, an estimation of the time needed to go from one point to another, namely the FPT, crucially depends on the confining environment—the mean FPT (MFPT) being actually infinite in unbounded domains.

Consider a random walker moving in a bounded domain of size N. Let $W(\mathbf{r}, t|\mathbf{r}')$ be the propagator (that is, the probability density of being at site $\mathbf{r}$ at time t, starting from site $\mathbf{r}'$ at time 0), and $P(\mathbf{r}, t|\mathbf{r}')$ the probability density that the FPT to reach $\mathbf{r}$, starting from $\mathbf{r}'$, is t. These two probability densities are known to be related through[23]

$$W(\mathbf{r}_{\mathrm{T}},t|\mathbf{r}_{\mathrm{S}})=\int_0^t P(\mathbf{r}_{\mathrm{T}},t'|\mathbf{r}_{\mathrm{S}})W(\mathbf{r}_{\mathrm{T}},t-t'|\mathbf{r}_{\mathrm{T}})\mathrm{d}t' \quad (1)$$

where $\mathbf{r}_{\mathrm{S}}$ and $\mathbf{r}_{\mathrm{T}}$ denote, respectively, the source and target position. After integration over t, this equation gives an exact expression for the MFPT, provided it is finite:

$$\langle \mathbf{T}\rangle = \frac{H(\mathbf{r}_{\mathrm{T}}|\mathbf{r}_{\mathrm{T}})-H(\mathbf{r}_{\mathrm{T}}|\mathbf{r}_{\mathrm{S}})}{W_{\mathrm{stat}}(\mathbf{r}_{\mathrm{T}})} \quad (2)$$

where

$$H(\mathbf{r}|\mathbf{r}')=\int_0^\infty (W(\mathbf{r},t|\mathbf{r}')-W_{\mathrm{stat}}(\mathbf{r}))\mathrm{d}t \quad (3)$$

and W_{stat} is the stationary probability distribution (see Supplementary Information for details). Equation (2) is an extension of an analogous form given in ref. 24, for which no quantitative determination of the MFPT could be proposed. The main problem at this stage is to determine the unknown function H, which is indeed a complicated task, as it depends both on the walk's characteristics and on the shape of the domain. A crucial step that allows us to go further in the general case is that H turns out to be the pseudo-Green function of the domain[25], which in turn is well suited to a quantitative analysis. Indeed, we propose approximating H by its infinite-space limit, which is precisely the usual Green function G_0:

$$H(\mathbf{r}|\mathbf{r}')\approx G_0(\mathbf{r}|\mathbf{r}')=\int_0^\infty W_0(\mathbf{r},t|\mathbf{r}')\mathrm{d}t \quad (4)$$

where W_0 is the infinite space propagator (Supplementary Information). Note that a similar approximation has proven to be satisfactory in the standard example of regular diffusion[26]. We stress that when inserted in equation (2), this form does not lead to a severe infinite space approximation of the MFPT, because all the dependence on the domain geometry is now contained in the factor $1/W_{\mathrm{stat}}$. This approximation is the key step of our derivation and, as we proceed to show, captures extremely well the confining effects on MFPTs in complex media.

We first consider the case of a uniform stationary distribution $W_{\mathrm{stat}}=1/N$, which is realized as soon as the links of the network are not directed and the number of connected neighbours of a node, the degree, is constant. This assumption amounts to symmetrical transition rates and actually underlies many models of transport in complex media, with the notable exception of scale-free networks, which will be tackled later on in this Letter. Following ref. 3, we assume for W_0 the standard scaling:

$$W_0(\mathbf{r},t|\mathbf{r}')\propto t^{-d_{\mathrm{f}}/d_{\mathrm{w}}}\Pi\left(\frac{|\mathbf{r}-\mathbf{r}'|}{t^{1/d_{\mathrm{w}}}}\right) \quad (5)$$

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where the fractal dimension d_f characterizes the number of sites $N_r \propto r^{d_f}$ within a sphere of radius r, Π is the infinite space scaling function, and d_w has been defined previously. This form ensures the normalization of W_0 by integration over the whole fractal set. A derivation given in Supplementary Information then yields our central result:

$$\langle \mathbf{T} \rangle \sim \begin{cases} N(A - Br^{d_w - d_f}) & \text{for } d_w < d_f \\ N(A + B\ln r) & \text{for } d_w = d_f \\ N(A + Br^{d_w - d_f}) & \text{for } d_w > d_f \end{cases} \qquad (6)$$

for $r = |\mathbf{r}_T - \mathbf{r}_S|$ different from 0; here '$\sim$' indicates large N asymptotic equivalence. Strikingly, the constants A and B do not depend on the confining domain. In addition, whereas A is related to the small-scale properties of the walk, we emphasize that B can be written solely in terms of Π (a precise definition of A and B is given in Supplementary Information). These expressions therefore unveil a universal scaling dependence of the MFPT on the geometrical parameters N and r.

Several comments are in order. First, we point out that equation (6) gives the large N asymptotics of the MFPT, which is a function of N and r as independent variables. In particular, the volume dependence is linear in N for r fixed in any case, which can not be inferred from the standard scaling $\langle \mathbf{T} \rangle \propto L^{d_w}$, L being the characteristic length of the domain of order N^{1/d_f}. Second, a global rescaling of the problem $r \to \lambda r$, $L \to \lambda L$, when applied to equation (6), gives the standard form $\langle \mathbf{T} \rangle \propto \lambda^{d_w}$ for $d_w > d_f$ and $\langle \mathbf{T} \rangle \propto \lambda^{d_f}$ for $d_w < d_f$ in accord with refs 27 and 28. Third, equation (6) shows two regimes, which rely on infinite space properties of the walk: in the case of compact exploration[3] ($d_w \geq d_f$) where each site is eventually visited, the MFPT behaves like $\langle \mathbf{T} \rangle \propto Nr^{d_w - d_f}$ ($\langle \mathbf{T} \rangle \propto N \ln r$ for $d_w = d_f$) at large distances, so that the dependence on the starting point always matters; in the opposite case of non-compact exploration, $\langle \mathbf{T} \rangle$ tends to a finite value for large r, and the dependence on the starting point is lost.

We now confirm these analytical results by Monte Carlo simulations and exact enumeration methods applied to various models that exemplify the three previous cases. (1) The random barrier model in two dimensions[3] is a widespread model of transport in disordered systems in which MFPT properties remain widely unexplored. It is defined by a lattice random walk with nearest neighbours symmetrical transition rates Γ distributed according to some distribution $\rho(\Gamma)$. Even for a power law distribution $\rho(\Gamma)$ the scaling function $\Pi(\xi)$ can be shown to be gaussian[10] ($d_f = d_w = 2$), which allows us to explicitly compute the constant B and obtain $\langle \mathbf{T} \rangle \sim N(A + (1/2\pi D_{eff})\ln r)$. Here D_{eff} is a diffusion constant depending on $\rho(\Gamma)$ that can be determined by an effective medium approximation[10] (Supplementary Information). (2) The Sierpinski gasket of finite order is a representative example of deterministic fractals, described in Fig. 1. In this case[3] $d_f = \ln 3/\ln 2 < \ln 5/\ln 2 = d_w$, so that our theory predicts the scaling $\langle \mathbf{T} \rangle \propto Nr^{(\ln 5 - \ln 3)/\ln 2}$. (3) The Lévy flight model of anomalous diffusion[11,23] is based on a fat-tailed distribution of jump lengths $p(l) \propto l^{-d-\beta}$ ($0 < \beta \leq 2$). The walk dimension is now $d_w = \beta$, whereas the fractal dimension is the dimension of the euclidian space d. In dimensions $d \geq 2$, or for $d = 1$ when $\beta < 1$, one has $d_f > d_w$ and our theory gives $\langle \mathbf{T} \rangle \sim N(A - Br^{\beta - d})$.

Figure 2a–c reveals excellent quantitative agreement between the analytical predictions and the numerical simulations. Both the volume dependence and the source–target distance dependence are unambiguously captured by our theoretical expressions, equation (6), as shown by the data collapse of the numerical simulations. We emphasize that the very different nature of these examples demonstrates that the range of applicability of our approach, which mainly relies on the length-scale-invariant property of the infinite space propagator (equation (5)), is wide.

These analytical results can be extended to scale-free networks. The latter are characterized by a power-law degree distribution. A wide class of scale-free networks has been proven recently to be invariant under a length-scale renormalization scheme defined in ref. 15: social networks[20], the world wide web[29], metabolic networks[22], and yeast protein interaction networks (PIN)[21]. Although the standard fractal dimension d_f of these networks is infinite as their diameter scales as $\ln N$, one can show that they are scale-invariant in the following sense: they can be covered with N_B non-overlapping boxes of size l_B with $N_B/N \propto l_B^{-d_B}$. This renormalization property defines an alternative scaling exponent called the box dimension d_B, which is actually equal to the fractal dimension defined earlier as long as the networks are not of small-world type. A model of scale-free networks possessing such length-scale-invariant properties has been defined recursively in refs 12 and 30: the network grows by adding m new offspring nodes to each existing network node, resulting in well defined modules. In addition, modules are connected to each other through x random links (Supplementary Information). In this case $d_B = \ln(2m + x)/\ln 3$ and $d_w = \ln(6m/x + 3)/\ln 3$.

For this class of networks, $W_{stat}(\mathbf{r})$ is not uniform any more but proportional to the degree $k(\mathbf{r})$ of the node $\mathbf{r}$. One can use the length-scale-invariant property to infer the following scaling of the infinite space propagator:

$$\frac{W_0(\mathbf{r},t|\mathbf{r}')}{k(\mathbf{r})} \propto t^{-d_B/d_w}\,\Pi\left(\frac{|\mathbf{r}-\mathbf{r}'|}{t^{1/d_w}}\right) \qquad (7)$$

This form, compatible with the symmetry relations proposed in ref. 24, allows us to perform a similar derivation, which leads for the MFPT to the same result (equation (6)), but where d_f is to be replaced

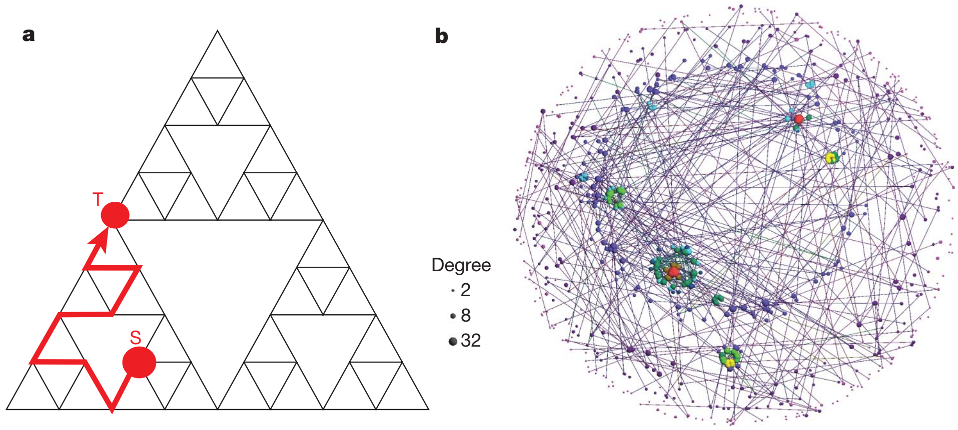

Figure 1 | Length-scale-invariant networks. a, The Sierpinski gasket (here of order three) is a representative example of a deterministic fractal. A sample random path from S to T is shown. **b**, The yeast PIN, obtained from the filtered yeast interactome developed in ref. 21. Picture generated by LaNet-vi software (http://xavier.informatics.indiana.edu/lanet-vi/).

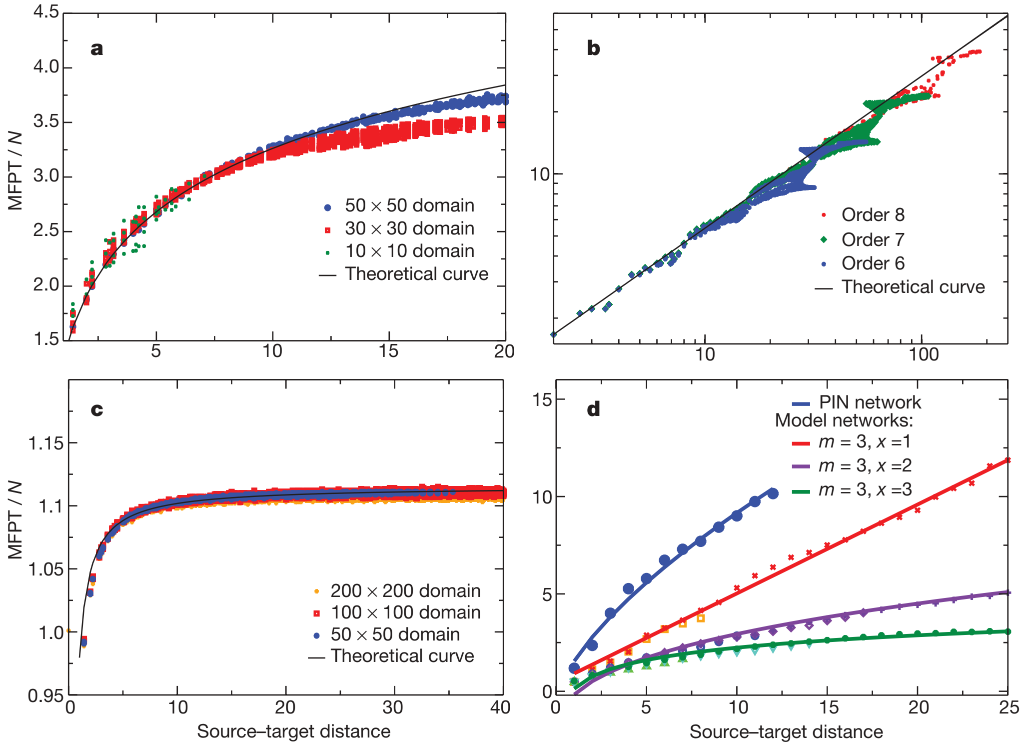

Figure 2 | Mean FPT in complex media. **a**, Random barrier model with a transition rate distribution $\rho(\Gamma)=(\alpha/\Gamma)(\Gamma/\Gamma_0)^{\alpha}$, with $\Gamma_0=1$ and $\alpha=0.5$. The confining domain is an $L\times L$ square with the target point in the middle. Shown are numerical simulations of the MFPT rescaled by the volume N, averaged over the disorder, for three different domain sizes. The theoretical curve (black line) is given by $\langle \mathbf{T}\rangle/N\sim(A+(1/2\pi D_{\text{eff}})\ln r)$, where the only fitting parameter is A; D_{eff} is evaluated in Supplementary Information. **b**, Numerical simulations of random walks on a Sierpinski gasket (log/log plot) for three different system sizes (orders 6, 7 and 8). For each set of points, the size of the Sierpinski gasket and the target point are fixed (the target point corresponds to the point T on the Sierpinski gasket of order 3 in Fig. 1a, and the starting point takes various positions on the Sierpinski gasket). The black line corresponds to the theoretical scaling $r^{d_w-d_f}$. **c**, Simulations of Lévy flights on a two-dimensional square lattice ($\beta=1$). The confining domains are 50×50, 100×100 and 200×200 squares, with the target in the middle. The MFPT is presented as a function of the source–target distance for different source points. Simulation points are fitted with $\langle \mathbf{T}\rangle/N\sim(A-Br^{\beta-2})$. **d**, Simulations of random walks on fractal complex networks of small-world type. The MFPT on the PIN network (blue circles) is fitted by $\langle \mathbf{T}\rangle/N\sim(A+Br^{d_w-d_B})$ with $d_w\approx2.86$ and $d_B\approx2.2$, as found in ref. 12. We also consider three examples of the model of networks defined in ref. 12: ($m=3, x=1, d_B-d_w=1$), red symbols and fitting curve; ($m=3, x=2, d_B-d_w=\ln(3/2)/\ln3$), violet symbols and fitting curve; and ($m=3, x=3, d_B-d_w=0$), green symbols and fitting curve. For each example, the MFPT (rescaled by the network volume $N=(1+x)^k$ for three system sizes $k=3, 4, 5$) averaged over the disorder is presented as a function of the source–target distance for different source points, and fitted by the theoretical expression $\langle \mathbf{T}\rangle/N\sim(A+Br^{\ln(3/x)/\ln3})$. We find quite surprisingly a scaling independent of m.

by d_B. We applied this formula to an example of a scale-free biological network, the yeast PIN (Fig. 1b), obtained from the filtered yeast interactome developed in ref. 21, and to a model[12,30] of a scale-free fractal network. Figure 2d shows that this analytical result is in good agreement with numerical simulations on the PIN network. The data collapse over various system sizes for the model of scale-free fractal networks provides a further validation of our approach, and indicates that our theory has a wide range of applications.

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Supplementary Information is linked to the online version of the paper at www.nature.com/nature.

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