25th ABCM International Congress of Mechanical Engineering
October 20-25, 2019, Uberlândia, MG, Brazil

COBEM-2019-0367
WORKFLOW FOR DIGITAL PETROPHYSICS WITH RANDOM WALK

Danilo Jose da Silva
Alexandre Zabot
James Eger
Universidade Federal de Santa Catarina, Centro Tecnológico de Joinville, Joinville, Brasil.
danilo.s@grad.ufsc.br
alexandre.zabot@ufsc.br
james.eger@ufsc.br

Abstract. *We present a workflow to obtain the transport properties (Permeability, Surface by Volume and Tortuosity) of a porous medium by means of Random Walk Simulation (RWS)(Silva* et al.*, 2017). A methodology that is able to extract the transport properties of the porous medium by random particle walking (Nakashima and Watanabe, 2002). The method that is initially described by Nakashima and Watanabe (2002) is applied by the author, in a sample of artificial rock, which is composed of a set of regular spheres, where the description of the obtained results showed very promising data. Later, Silva* et al. *(2017) validates this method, but now applied to real rock samples (Sandstone and Carbonate), because it has a simple implementation, the methodology requires a low computational cost and the results are expressive when compared to the already used tools in the area.*

Key Words: *Random Walk, Digital Rock, Porous Media, Transportation Properties, Mean Maximal Excursion.*

1. INTRODUCTION

Well established Methods such as the Lattice Boltzman Method (LBM) to obtain porous media transport properties present a precise invasion description thus obtaining transport properties close to the experimental ones. The Young-Laplace Method (YLM) (Hazlett, 1995; S. Magnani *et al.*, 2000; Hilpert and Miller, 2001; G Wolf *et al.*, 2013) it's a fast simulation method because it simplifies the problem physics of the flow in porous media, considering only the invasion front geometry and has a great advantage because it can simulate any type of geometry no matter how complex. LBM (Qian *et al.*, 1992; Chen *et al.*, 1992) can also simulate any type of complex geometry but with the advantage of simulating flow dynamics, a task that YLM cannot accomplish. However, such techniques have a high computational cost.

The RWS is an alternative method described in the literature, which obtains the transport properties *(Permeability, Surface by Volume and Tortuosity)* by means of the random walk of particles (Nakashima and Watanabe, 2002). The methodology, requires a small simulation time when compared to the LBM. The method consists in throw in walkers into a porous medium that, as they travel, "map" the digital rock. Nakashima and Watanabe (2002) presented the method in the literature applied to an artificial rock sample, in which its structure is composed of a set of regular spheres, and the results of the publication were very promising and with a reasonable simulation time.

The study article: "Random Walk in Petrophysics" (Silva *et al.*, 2017) is a validation of the method, however this time it is applied to real rocks (Raeini *et al.*, 2017). Silva *et al.* (2017), however, is limited only to presenting the results for comparison with other methods already disseminated in the area. In this manuscript, we will present a workflow with a sequence of steps, in order to show the achievement of the results present in Silva *et al.* (2017).

2. PARAMETERS OF DIGITAL PETROPHYSICS

2.1 Random Walk

Each walker starts from a random position in the digital rock, with discrete movement times (where τ is adopted as discrete time for each walker's displacement) (Nakashima and Watanabe, 2002). The walker is allowed to move only one voxel-pore at a time. The walker must respect the geometry limits and the solid voxels. When the direction drawn is a voxel-solid, the particle must remain motionless and wait for the next step to draw a new direction. The mean squared displacement for n walkers is (Nakashima and Watanabe, 2002; Tejedor *et al.*, 2010):

$$\left\langle \vec{r}^{\,2}(\tau) \right\rangle = \frac{1}{n} \sum_{i=1}^{n} \vec{r}_i^{\,2}(\tau) \tag{1}$$

Each particle starts from a random origin in the rock (Fig. 1(a)), traversing only the voxels pore (blank), respecting the limits of the rock and voxels solid (gray). Movement occurs only in the first neighbors nearby.

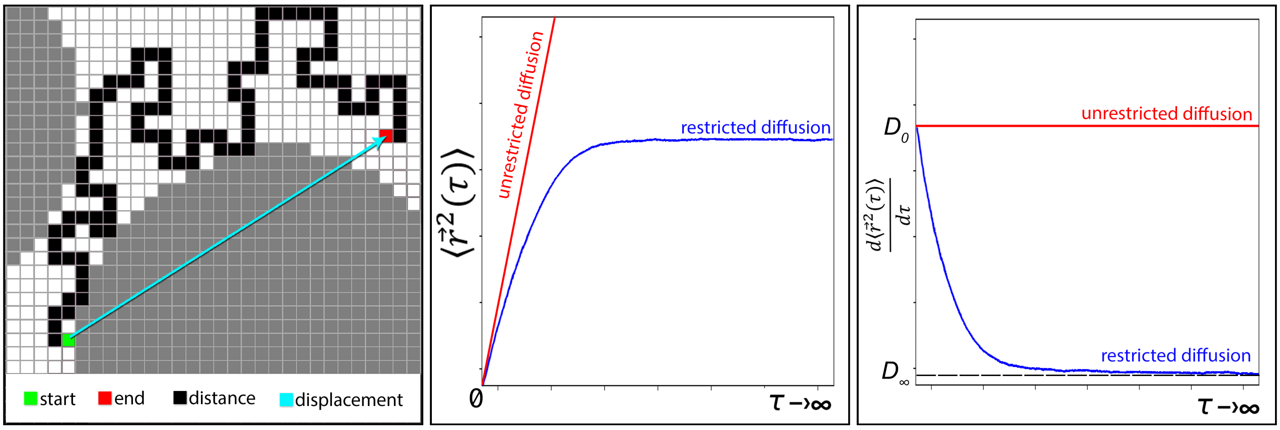

Figure 1. (a) Walk of a Particle in a 2D Medium. (b) Mean Square Displacement. (c) Numerical Derivative of Fig. 1(b).

For a fully porous medium ($\phi = 1$) the mean square displacement will have a linear behavior (Fig. 1b). In real cases, where voxels solids and voxels pores are present, this behavior becomes a curve because walkers are in a confined space (rock boundary and solid voxels) which causes flattening of the curve (Fig. 1(b): restricted diffusion).

2.2 Coefficient of Diffusion

According to Nakashima and Watanabe (2002) the diffusion coefficient in a three-dimensional space is given by the temporal derivatives of the mean quadratic displacement:

$$D(t) = \frac{1}{6} \frac{d\left\langle r^2(t) \right\rangle}{dt} \tag{2}$$

We can approximate the numerical derivative of the mean squared displacement (Ibe, 2013) by:

$$\frac{d\left\langle \vec{r}^{\,2}(\tau) \right\rangle}{d\tau} \approx \left\langle \vec{r}^{\,2}(\tau) \right\rangle - \left\langle \vec{r}^{\,2}(\tau+1) \right\rangle \tag{3}$$

Finally:

$$D(\tau) \approx \frac{1}{6} \left[\left\langle \vec{r}^{\,2}(\tau) \right\rangle - \left\langle \vec{r}^{\,2}(\tau+1) \right\rangle \right] \tag{4}$$

2.3 Curve Fitting

We obtain the transport parameters by means of a curve fit. Using the equation described in Nakashima and Watanabe (2002) and applying the necessary simplifications (Silva *et al.*, 2017) we have:

$$y = y_0 \left(1 - a\sqrt{\tau} + b\tau\right) \qquad for\ \tau \to 0 \tag{5}$$

where: $a = \frac{4}{9\sqrt{\pi}} \left(\frac{S}{V}\right)_{pore} \sqrt{D_0}$; $b = c_1$ e $y_0 = D_0$.

Therefore, the *Surface by Volume* of the pores $\left(\frac{S}{V}\right)_{pore}$ will be:

$$\left(\frac{S}{V}\right)_{pore} = \frac{9\sqrt{\pi}a}{4\sqrt{D_0}} \tag{6}$$

We estimate the *Permeability* with an approximation of the Kozeny-Carman relation (Nakashima and Watanabe, 2002; Tiab and Donaldson, 2003):

$$k \approx \frac{\phi}{\left(\frac{D_0}{D_\infty}\right)\left(\frac{S}{V}\right)^2_{pore}} \tag{7}$$

where: ϕ is the porosity, D_∞ is the asymptote and $\left(\frac{D_0}{D_\infty}\right)$ it's the *Tortuosity*.

3. WORKFLOW

3.1 Number of Walkers

It is necessary to have a large number of walkers for the curve of the mean square displacement to have statistical significance and so that all voxels pore are visited. We can determine a minimum number of walkers casting a single walk in the porous medium of interest to estimate a percentage of the pores visited. According to the Fig. 2(a) we noticed a linear relationship between the percentage visited pores and τ. Therefore two simulations are sufficient to estimate the number of initial walkers to visit all the porous medium.

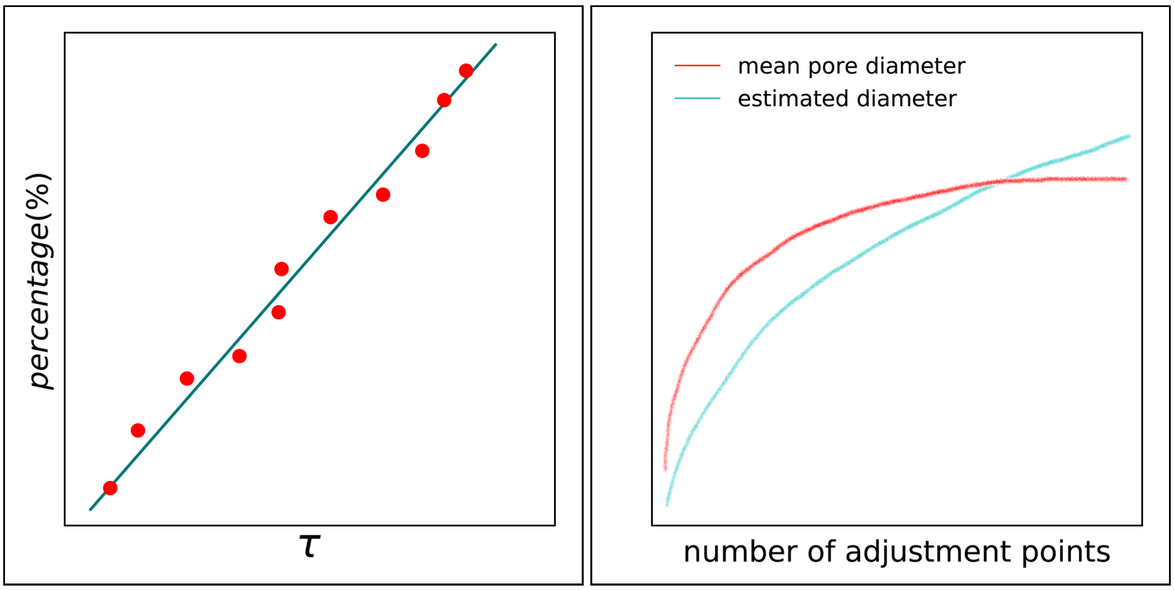

Figure 2. (a) Graph that relates τ with the percentage visited voxels pore. (b) Graph of the *mean pore diameter* (D_{mp}) and *estimated pore diameter* (D_{ep}) in function of the number of points in fitting.

In Fig. 2(a) it is important to be attentive of the connectivity between the rock pore-voxels, because as the connectivity decreases the points become more dispersed and consequently less reliable.

3.2 Number of steps to cross the rock

The method of *Mean Maximal Excursion (MME)* provides the longest distance r that a random walker reaches up to one τ (Tejedor *et al.*, 2010). We want the average maximum distance traveled by the random walker, considering a process of diffusion "normal" (Krapf, 2015):

$$\langle r \rangle = \frac{\Gamma(\frac{4}{2})}{\Gamma(\frac{3}{2})}\sqrt{4D\tau} \tag{8}$$

where: D is the diffusion coefficient, which values $1/6$ in 3D (Yuste *et al.*, 2001). Therefore:

$$\langle r \rangle = \frac{\Gamma(\frac{4}{2})}{\Gamma(\frac{3}{2})}\sqrt{\frac{2\tau}{3}} \approx 0.9\sqrt{\tau} \tag{9}$$

Finally, for a cube with edge "l" the diagonal is $r = \sqrt{3}l$. With the Eq. (9) we get the typical number of steps for the walkers to cross the diagonal:

$$\tau \approx 4l^2 \tag{10}$$

By experience, the Eq. (10) in most cases it is effective in identifying where the characteristic flattening of the curve begins. In order to achieve an acceptable asymptotic behavior, a safety margin is adopted based on the various simulations performed, then the Eq. (10) it becomes:

$$\tau \approx 3(4l^2) \tag{11}$$

3.3 Number of Points for Curve Fitting

For good curve fitting (Section 2.3) it is necessary to provide a satisfactory number of points. According to the Eq. (5) the adjustment must be applied to a τ sufficiently small which is typically the time while the walker is within the pore of origin. If τ_p is the typical length of time that the walker stays within the pore, using the Eq. (10) the estimated pore diameter will be $D_{ep} \approx \sqrt{\frac{\tau_p}{4}}$. On the other hand, adjusting the data in Eq. (5) we obtain that the $(\frac{S}{V})_{pore}$ is directly related to the mean diameter of the pore if we consider it as spherical:

$$\left(\frac{S}{V}\right)_{pore} = \frac{4\pi {R_{mp}}^2}{\frac{4}{3}\pi {R_{mp}}^3} = \frac{3}{R_{mp}} = \frac{6}{D_{mp}} \quad \therefore \quad D_{mp} = \frac{6}{\left(\frac{S}{V}\right)_{pore}} \tag{12}$$

When τ_p is correct, the two diameters must match. Since we do not know a priori the value of τ_p, we make several adjustments and we obtain a graph of the two diameters in function of the several τ_p used. The intersection of curves (Fig. 2b) gives us the correct τ_p.

4. WORKFLOW APPLICATION

The method was applied for Ketton Carbonate rock, the digital rock has dimensions 1000^3 voxels, with a resolution of 3,0001 (μm) and porosity $\phi = 0.132$, the rock and data are described in Raeini *et al.* (2017).

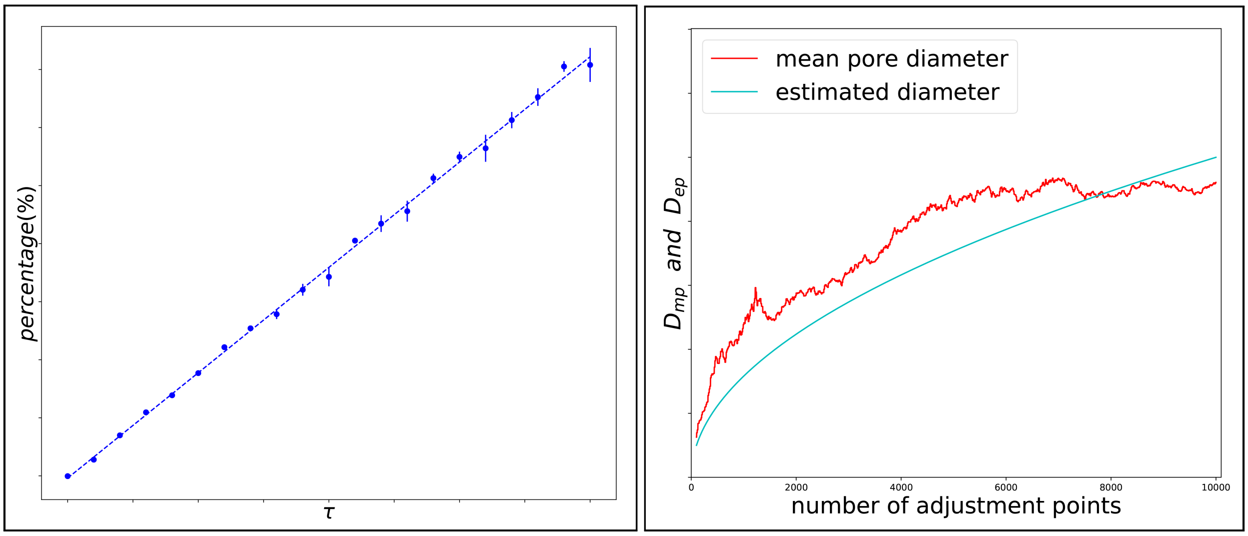

Figure 3. (a) Percentage traveled on voxels-poro as a function of τ. (b) *Mean pore diameter* (D_{mp}) and *Estimated pore diameter* (D_{ep}) in function of the number of points in fitting.

By following Section 3.1 it is possible to arrive at the minimum number of walkers across the generated line, Fig. 3(a) will be an initial parameter for defining a reasonable number of walkers in order to obtain a pore representativeness.

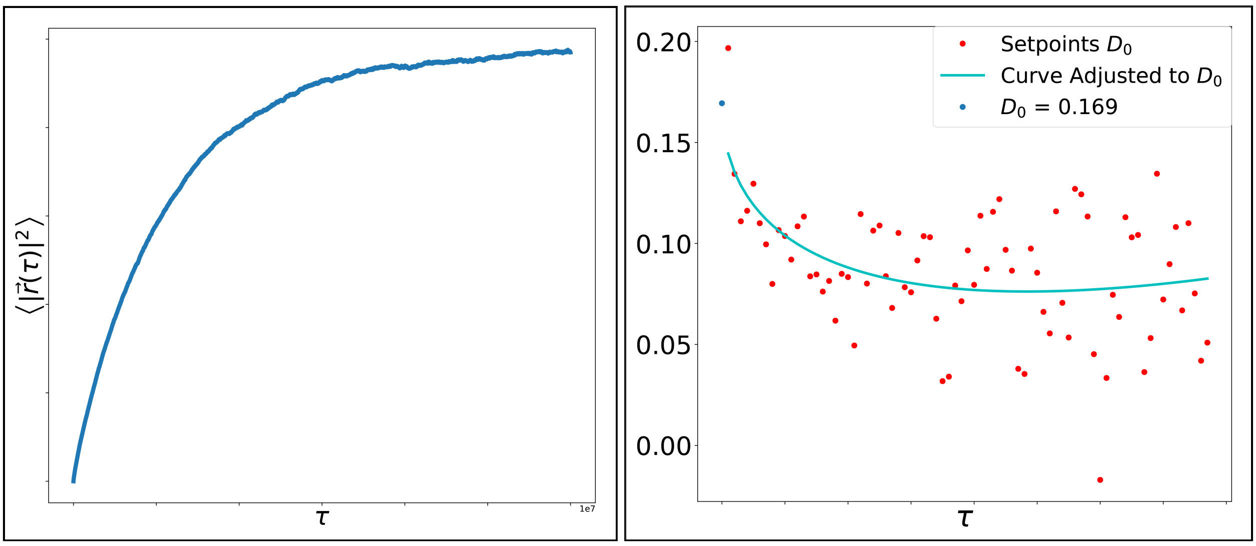

Figure 4. (a) Mean Square Displacement in function of τ. (b) Curve fitting by Eq. (5).

Using Eq. (11) for digital rock simulation it is noticeable that the calculated value is sufficient for the curve to achieve its asymptotic behavior (Fig. 4(a)) thus indicating that most walkers explored the entire digital rock. Applying the definition of numerical derivative in Fig. 4(a) and obtaining Fig. 3(b), we arrive at the number of adjustment points which consequently gives us the D_0. Applying D_0 on Eq. (6) gives one of the transport properties (*Surface by Volume*). Fig. 4(b) because it is a derivative in discrete times, the lack of homogeneity in the curve generates a difference that impacts the final result, and of course the more significant the number of walkers, the smaller the point cloud dispersion, and therefore a greater representation of the porous medium of study. For *Tortuosity* and *Permeability* it is necessary to find D_∞. It is obtained by applying the definition of numerical derivative to Fig. 4(a) before flattening, that is, when it still has a straight line behavior.

5. CONCLUSIONS

As mentioned, the number of initial walkers should be measured by two initial simulations with a reasonable τ, and as shown in Fig. 2(a) this walk behaves linearly as τ increases. The ratio of: *voxels pore traveled / total pore voxels*, gives us the two points and consequently their slope. It is important to note that as *voxel pore connectivity* decreases, these points become less reliable as in confined regions the hiker is limited to a short space, often leaving him in the same location to meet the established RWS criteria, thus increasing the margin of error in the line slope.

In calculating the D_∞ as already mentioned, its, is obtained by applying the definition of numerical derivative in Fig. 4(a) when it is still a straight line. Its value is obtained by the simple average of the last points, where this quantity is a criterion to be defined based on a representative quantity of points. The criterion adopted by Silva *et al.* (2017) is 10% of the total points when the curve is still a straight line. The results obtained for the transport properties $(Permeability, Tortuosity\ and\ Volume\ Surface)$ showed promising data, with a reasonable margin of error for Tortuosity and Volume Surface. The obtained data, and comparisons with the other methods can be consulted in Silva *et al.* (2017).

6. ACKNOWLEDGMENTS

Author is greatly indebted to Brazilian Petroleum Company (Petrobras) for the financial support.

7. REFERENCES

Chen, H., Chen, S. and Matthaeus, W.H., 1992. "Recovery of the navier-stokes equations using a lattice-gas boltzmann method". *Phys. Rev. A*, Vol. 45, pp. R5339–R5342. doi:10.1103/PhysRevA.45.R5339. URL https://link.aps.org/doi/10.1103/PhysRevA.45.R5339.

G Wolf, F., Zabot, A., O Emerich, L. and Santos, D., 2013. "Deslocamento imiscÍvel em poros de duplo canal: Uma comparaÇÃo entre modelos dinÂmicos e quase-estÁticos".

Hazlett, R.D., 1995. "Simulation of capillary-dominated displacements in microtomographic images of reservoir rocks". *Transport in Porous Media*, Vol. 20, pp. 21–35.

Hilpert, M. and Miller, C.T., 2001. "Pore-morphology-based simulation of drainage in totally wetting porous media".

Ibe, O.C., 2013. *Elements of random walk and diffusion processes*. Wiley series in operations research and management science. Wiley. ISBN 9781118618059,111861805X,9781118629857,111862985X,978-1-118-61809-7. URL http://gen.lib.rus.ec/book/index.php?md5=b5789369a4824b7d22d868fdcd451aad.

Krapf, D., 2015. "Chapter five - mechanisms underlying anomalous diffusion in the plasma membrane". In A.K. Kenworthy, ed., *Lipid Domains*, Academic Press, Vol. 75 of *Current Topics in Membranes*, pp. 167 – 207. doi:https://doi.org/10.1016/bs.ctm.2015.03.002. URL http://www.sciencedirect.com/science/article/pii/S1063582315000034.

Nakashima, Y. and Watanabe, Y., 2002. "Estimate of transport properties of porous media by microfocus x-ray computed tomography and random walk simulation". *Water Resources Research*, Vol. 38, No. 12, pp. 8–1–8–12. doi:10.1029/2001WR000937. URL https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2001WR000937.

Qian, Y.H., DHumières, D. and Lallemand, P., 1992. "Lattice BGK models for navier-stokes equation". *Europhysics Letters (EPL)*, Vol. 17, No. 6, pp. 479–484.

Raeini, A.Q., Bijeljic, B. and Blunt, M.J., 2017. "Generalized network modeling: Network extraction as a coarse-scale discretization of the void space of porous media". *Phys. Rev. E*, Vol. 96, p. 013312. doi:10.1103/PhysRevE.96.013312. URL https://link.aps.org/doi/10.1103/PhysRevE.96.013312.

S. Magnani, F., Philippi, P., Liang, Z. and P. Fernandes, C., 2000. "Modelling two-phase equilibrium in three-dimensional porous microstructures". *International Journal of Multiphase Flow - INT J MULTIPHASE FLOW*, Vol. 26, pp. 99–123. doi:10.1016/S0301-9322(99)00008-7.

Silva, D., Zabot, A. and Siebert, D., 2017. "Random walk in petrophysics". doi:10.26678/ABCM.COBEM2017.COB17-0820.

Tejedor, V., Bénichou, O., Voituriez, R., Jungmann, R., Simmel, F., Selhuber-Unkel, C., Oddershede, L.B. and Metzler, R., 2010. "Quantitative analysis of single particle trajectories: Mean maximal excursion method". *Biophysical Journal*, Vol. 98, No. 7, pp. 1364 – 1372. ISSN 0006-3495. doi:https://doi.org/10.1016/j.bpj.2009.12.4282. URL http://www.sciencedirect.com/science/article/pii/S0006349509060974.

Tiab, D. and Donaldson, E., 2003. *Petrophysics: Theory and Practice of Measuring Reservoir Rock and Fluid Transport Properties: Second Edition*, p. 1008. ISBN 9780123838483.

Yuste, S.B., Acedo, L. and Lindenberg, K., 2001. "Order statistics for d-dimensional diffusion processes". *Phys. Rev. E*, Vol. 64, p. 052102. doi:10.1103/PhysRevE.64.052102. URL https://link.aps.org/doi/10.1103/PhysRevE.64.052102.

8. RESPONSIBILITY NOTICE