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Parameter calibration between models and simulations: Connecting linear and non-linear descriptions of anomalous diffusion

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HIGHLIGHTS

- The curves of the Figs. 5 and 6 have were modified to become more visible.
- English language edition was performed in the manuscript.
- Motivated by this edition, the title of the article has been changed for "Parameter calibration between models and simulations: connecting linear and non-linear descriptions of anomalous diffusion".

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ABSTRACT

Anomalous diffusion is an ubiquitous phenomenon which have been studied by several approaches, including simulation, analytical methods and experiments. Partial differential equations, either fractional linear ones as non-linear, are able to describe the phenomenon, in particular, the heavy tails observed in the probability distribution functions. Besides, one can observe some difficulties to tame the anomalous diffusion parameters in many simulations studies. Consequently, the relationship between simulations results to the corresponding model becomes somewhat impaired. In this work, we present a systematic calibration between simulations and models, exploring the relationship among the diffusion coefficients and diffusion exponents with the order of fractional derivatives, q-Gaussian parameter and model diffusion constant. By means of a statistical fitting procedure of the simulations data, we establish a connection between linear and non-linear approaches. Simulations considered a CTRW with a criterion to control mean waiting time and step length variance, and a full range of well controlled cases ranging from subdiffusion to superdiffusion regimes were generated. Theoretical models were expressed by means of generalised diffusion equations with fractional derivatives in space and time and by the non-linear porous medium equation. To assess the diffusion constant, the order of fractional derivatives and the q-Gaussian parameter of simulations data in each case of anomalous diffusion, we compare the accuracy of two methods: (1) by analysis of the dispersion of the variance over time and, (2) by the optimisation of solutions of the theoretical models to the histogram of positions. The relative accuracies of the models were also analysed for each regimen of anomalous diffusion. We highlight relations between

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simulations parameters and model parameters and discuss methods to link them. Among those, Tsallis–Buckman scaling law was verified.

1. Introduction

Systems with large numbers of particles subject to short range interactions tend to exhibit Brownian motion at small scale and classical diffusion behaviour at large scale [1]. However, a large plethora of natural phenomena with more complex detailed dynamics of the particles displays anomalous Brownian motion in small scale and, consequently, anomalous diffusion behaviour at small scale. Examples are: transport in turbulent plasma [2], anomalous diffusion of proteins [3,4], population dynamics [5–7], porous medium systems [8], diffusion in fractal structures [9], liquid crystals [10] and organisms [11]. In some recent efforts to simulate anomalous diffusion systems, it is possible to perceive certain difficulty in controlling the process in reproducing different regimes of anomalous diffusion [3,12–15]. As consequence, the choice of anomalous diffusion models to perform controlled simulations may be impaired. To obtain suitable simulations, it would be of interest to establish a systematic calibration between simulations and theoretical models. For that purpose, it turns necessary to take in account the many scales involved in the phenomena.

At small scale, the deviations from the classical Brownian motion may occur due to long range correlations between moving particles and/or with the background environment [16]. The particles in anomalous Brownian motion may have its displacements influenced through interactions with the background. According to local states of the background, the particle may experiment significantly high probabilities of having larger or smaller jumps than in the classical Brownian motion [17,18]. In special, in natural systems, the frequent occurrence of large jumps is commonly associated to heavy tails in the particle displacements probability distribution function (PDF), eventually displaying variance or mean not convergent. For instance, in ecological systems, the absence or abundance of food may regulate the length of displacement in the dispersal path of individuals of a given specie [19]. Moreover, the state of the background may impose to particles to be bounded to a site, in such manner that, the probabilities of observing long resting times between displacements is higher than the expected in classical case [20]. A typical example is the cage effect of molecules in a solvent [21,22]. Since the long range correlations are due the interaction of particles with the background, and not between the particles of interest, the large scale dynamic models are expected to be linear. Those process lies in the class of Lévy flights [17,23–25]. By the other hand, in some phenomena like diffusion in porous media, the position of the many neighbour particles influences the step size as well as the resting time of an individual particle, characterising long range interactions or correlations between the particles [26]. In such cases, since the correlations are between particles, it is expected that the associated dynamic models at large scale to be non-linear [27–29].

Turning our attention to a intermediary scale, it is assumed that the complex detailed dynamics at small scale can be summarised in the average parameters like particle mean resting time and the displacements variance. For a sufficiently large number of particles N, the particles displacements variance displays a power law dependence on time, $\langle X^2 \rangle \propto t^{\mu}$. Classical Brownian motion is associated with $\mu = 1$, whereas, if $\mu \neq 1$, it is associated to anomalous Brownian motion case, resulting in a more general class of anomalous diffusion at large scale [16,30]. If $\mu < 1$ the process is called subdiffusion and, for $\mu > 1$, superdiffusion.

The crossing from small scales to large scales is held when the sampling of the system becomes arbitrarily large. In the case of the classical Brownian motion, the large scale limit is described by the Central Limit Theorem (CLT). According to CLT, provided the convergence of population variance[1] is observed in the dynamics of a random variable at small scale, then the large scale sum of those variables will be Gaussian distributed. However, if the condition on the finite variance is not fulled, the resulting class of PDFs can be broadened [31]. Generalisations of the CLT are obtained with weaker conditions than the convergence in the average population. Among many generalisations of the CLT, there lies the Generalised CLT of Lévy–Gnedenko obtained from asymptotic conditions over power law distributions. In such case, the stable distribution in the limit of large number of particles is the Lévy distribution [32–34]. Alternatively, the q-Gaussian CLT, at the limit of large number of variables, exhibits as the stable distribution the q-Gaussian, provided conditions of convergence over the well defined q-mean and q-variance are verified [26,35]. In those cases, there may appears as a class of stable distribution, the so called heavy tailed distributions, for which, the population variance and, sometimes, the mean, becomes divergent.

At small scale limit, the particle positions PDF of the Brownian motion process is described by the diffusion equation [17,36]. However, in the anomalous Brownian case, the equations for the particle position PDF, as aforementioned, depends on characteristics of the complex processes at small scale. If the underlying particle dynamics has interactions, an example of model non-linear equation is the correlated diffusion equation (CDE), or porous medium equation, which corresponds to the case of interactions between particles [37]. In the linear case, the large scale description can be realised by fractional partial

[1] The distinction between sample and population averages is suitable since the mean and variance are calculated over a finite sample, whereas when calculated for the limiting distributions, the population averages may be divergent.