Introduction

1.1 Scope and introduction

In this thesis we are concerned with the simulation of fractional diffusion processes with and without central drift. We give discretizations by aid of explicit and implicit difference schemes. Then we use these discretizations, either for approximating the solution of the fractional diffusion equations or for the discrete random walks, obtained by the explicit difference scheme, for which we use the Monte Carlo method. The diffusion under the action of a central linear drift is a special case of the diffusion under the action of an external force. The partial differential equation modelling the motion of a bound particle under the action of an external force $F(x)$ is

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}\left(F(x)\, u(x,t)\right) \ , \qquad (1.1.1)$$

where a is the general positive constant of diffusion. In our notation $u(x,t)$ represents the probability density function. $F(x) = -\frac{dU(x)}{dx}$ where $U(x)$ is a symmetric differentiable potential, strictly increasing for $x > 0$. We consider $U(x)$ to represent either the quadratic harmonic oscillator, the quartic harmonic oscillator, or the mixed quadratic-quartic harmonic oscillator [10]. This equation is considered as a special form of the classical Fokker-Planck equation (see for example[86], [84], [82] and [53]) and also as a special form of the diffusion-convection equation (see for example [105], [110] and [99]). We distinguish also between the discrete solution of equation (1.1.1) as $F(x) = -x$ and the discrete generalized Ehrenfest model described by Vincze [107] and studied by many authors (see for example [92], [51],[6], [24], [4], and [7]).

We consider another important generalization of equation (1.1.1), namely we replace the first time derivative by the Caputo fractional derivative (see Appendix A) in order to obtain the time-fractional diffusion with central drift in the form

$$\frac{\partial^\beta u(x,t)}{\partial t^\beta} = a\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}(F(x)u(x,t)) \ , \ 0 < \beta \leq 1 \ , \qquad (1.1.2)$$

where a is the general diffusion constant. If $F(x) = -x$, we have the case of linear drift. We find the discrete approximations to the time-fractional diffusion processes with central drifts by devising the explicit and implicit difference schemes. We give the convergence of the discrete solutions as $t \to \infty$. Then by the Monte Carlo method we simulate the random walk of the models for different values of the time fractional order $\beta \in (0,1]$ [28] and [29]. It is worth to say that Metzler, Klafter and et al in [70], [71] and [3] refer to equation (1.1.2) as the fractional Fokker-Planck equation in their work with the anomalous diffusion and relaxation. See also [50], [2] and [100]. Gorenflo, Mainardi et al [40] have dealt with the discrete random walk solutions of the space-time fractional diffusion equation. We show in the treatment of the random walk the effect of the central drift $F(x)$ which enforces the diffusive particle to go back to the origin.

Actually the fractional calculus has gained great interest among mathematicians, physicists, engineers and biologists in recent years. The increasing popularity of fractional models has made fractional calculus a field of strong development in the last 30 years. The approximation of the fractional derivative operators is based on the discretization by the Grünwald-Letnikov scheme (see for examples Oldham & Spanier [79], Miller & Ross [72], Gorenflo & Mainardi [36], [35], [34], [40] and [27] and recently [62]).

In this thesis we discuss not only the discrete random walk but also the continuous time random walk (Montroll and Weiss 1965 [77]) for which the abbreviation CTRW is in common use. It is known that the CTRW can also be considered as a compound renewal process[13]. We focus our interest on random walks in which the probability distributions of the waiting times and jumps have fat tails characterized by power laws with exponent between 0 and 1 for the waiting times, between 0 and 2 for the jumps [30]. Gorenflo, Mainardi and et al [65] , [31], [37], [43] and [66] show that by starting from the relevant Lemmata (of Tauber type) the sojourn probability density of the random walker satisfies in the limit the fractional diffusion equation. We use here their successful methods for simulating the CTRW of fractional diffusion process and, by using a relevant transformation theorem [5] for the independent variables we simulate the CTRW of the space-fractional diffusion process with central linear drift

$$\frac{\partial v(\xi,\tau)}{\partial \tau} = b\frac{\partial}{\partial \xi}(\xi v(\xi,\tau)) + a\, {}_{\xi}D_{\theta}^{\alpha}\, v(\xi,\tau) \ , \ 0 < \alpha \leq 2 \ , \ v(\xi,\tau) = \delta(\xi) \ , \tag{1.1.3}$$

where $a > 0$ representing the diffusion constant and $b > 0$ representing the drift constant. We show in the simulation of this model how the initial position of particle plays an important role and how the central linear drift drives the diffusive particle towards the origin. We show that the space and the time scales of the diffusive particle under the action of central linear drift are compressed by the transformation theorem, see Section (4.5).

Since the fractional diffusion equation can be considered as a special case of equation (1.1.1) with $F(x) = 0$, we prove that the discrete solution of the space-time fractional diffusion equation tends in the limit, as the scaling factors of space and time tend to zero, to the Fourier-Laplace transform of the solution of equation (1.1.1). Gorenflo & Mainardi have proved the convergence of the discrete solution to the solution of the space-fractional diffusion equation [34]. In this thesis we generalize the proof to cover also the space-time fractional diffusion equation.

1.2 Organization of the thesis

In Chapter 2 we interpret the generalized Ehrenfest model as an explicit difference scheme and show the equivalence of its discretization to the discretization of the partial differential equation of diffusion with central linear drift (1.1.1). We calculate and plot the approximate solutions of this equation. We consider also the approximate solutions under the action of other forces. The convergence of the discrete solutions for time tending to infinity is discussed and plotted. The simulation exhibits exponential speed of convergence to the stationary solution of the discrete model, typical for an ergodic Markov chain. We simulate also the particle paths by the corresponding discrete random walks of these models.

In Chapter 3 we discuss the discrete solution of the time-fractional diffusion equation with central drift in a potential well (1.1.2). The discrete difference scheme shows that the particle remembers all its history, and this memory is also visible in the sketch of the particle paths. We calculate and plot the approximate solutions, the convergence for two different types of forces and for different values of the fractional order. Now the convergence to the stationary solution of the discrete model turns out as a power of t with negative exponent, hinting to a process with memory. We simulate also the path of the diffusive particle under the action of central linear drift by the aid of discrete random walks.

In Chapter 4 we give a survey on the theory of continuous time random walk. Then from the suitable choices of the waiting time and the jump densities we approximate the space-fractional diffusion process with central linear drift (1.1.3) through a suitable transformation of the independent variables of solution of space-fractional diffusion process without drift.

In Chapter 5 we complete our discussion of the fractional diffusion processes by proving that the discrete solution of these models tends in the limit as the space-time scaling factors tend to zero to the Fourier-Laplace transform of the solution of the fractional diffusion equations. We develop this theory for the time fractional diffusion equation and for the space-time fractional diffusion equation. Furthermore, we prove the convergence of the discrete solution of the time-fractional diffusion equation with central linear drift by proving that the discrete solution satisfies the same ordinary differential equation in Fourier-Laplace space.

In the Appendices A, B and C we give short surveys of the essentials of the fractional calculus, of stable probability distributions and of the Mittag-Leffler function, respectively.