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A Numerical study of Fractional Diffusion through a Langevin approach in random media

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Sommario

Lo studio del moto Browniano ha una lunga storia e coinvolge svariate formulazioni differenti. Tutte mostrano due risultati fondamentali: lo spostamento quadratico medio della particella che diffonde scala linearmente con il tempo e la densità di probabilità risulta essere una Gaussiana.

La diffusione standard in ogni caso non è universale. In letteratura ci sono numerose misure sperimentali [19] che mostrano une diffusione non lineare e non Gaussiana in molti campi come la fisica, la biologia, la chimica, l'ingegneria, l'astrofisica e altri. Questo comportamento può avere diverse origini fisiche ed è stato osservato frequentemente in sistemi spazialmente disordinati, in flussi turbolenti e in sistemi biologici con siti che legano le molecole o con affollamento macro-molecolare.

L'approccio di Langevin descrive il moto Browniano in termini di un'equazione stocastica differenziale. Il processo di diffusione è guidato da due parametri fisici, il tempo di rilassamento o correlazione τ e il coefficiente di diffusione della velocità D_v. In questo lavoro viene considerata una estensione di questo approccio ottenuta tramite l'introduzione di una popolazione di τ e D_v al fine di generare una dinamica frazionaria. Questo approccio si basa sull'idea che la diffusione frazionaria in mezzi complessi deriva da un processo Gaussiano con parametri random, dove queste caratteristiche random sono dovute alla complessità del mezzo. É stata realizzata una caratterizzazione statistica del mezzo complesso nel quale avviene la discussione ricavando le distribuzioni di questi parametri. Specifiche popolazioni di τ e D_v portano a particolari processi stocastici frazionari.

Questo approccio permette di preservare il moto Browniano classico come base ed è promettente per formulare processi stocastici per sistemi biologici che mostrano una dinamica complessa caratterizzata da diffusione frazionaria.

Lo studio numerico di questo approccio alternativo costituisce il presente lavoro di tesi.

Nel Capitolo 1 sono descritte le principali peculiarità della dinamica Browniana, sia per la particella libera che per una particella confinata da un potenziale armonico. Nel Capitolo 2 viene presentato un breve *excursus* riguardo altri modelli discussi in letteratura per la diffusione frazionaria, insieme alla descrizione delle sue caratteristiche fondamentali. Nel Capitolo 3 è riportata una descrizione del nuovo approccio bastato sull'equazione di Langevin per generare una cinetica frazionaria. In questo approccio la

superdiffusione si ottiene come generalizzazione della Langevin classica per una particella libera mentre per il caso subdiffusivo è necessario introdurre un potenziale confinante. Alcune dei risultati analitici presenti in questo Capitolo sono stati derivati da Silvia Vitali durante il suo periodo di ricerca all'estero presso il BCAM, Bilbao, sotto la supervisione del Dott. Gianni Pagnini. Nel Capitolo 4 vengono presentati i risultati numerici di questo approccio per il caso particolare della superdiffusione. In fine nell'Appendice sono riportate le definizioni di derivata frazionaria insieme ad alcune caratteristiche utili della funzione di Mainardi e delle distribuzioni stabili di Lévy.

Contents

Introduction

The study of Brownian motion has a long history and involves many different formulations. All these formulations show two fundamental common results: the mean square displacement of a diffusing particle scales linearly with time and the probability density function is a Guassian distribution.

However standard diffusion is not universal. In literature there are numerous experimental measurements [19] showing non linear diffusion in many fields including physics, biology, chemistry, engineering, astrophysics and others. This behavior can have different physical origins and has been found to occur frequently in spatially disordered systems, in turbulent fluids and plasmas, and in biological media with traps, binding sites or macro-molecular crowding.

Langevin approach describes the Brownian motion in terms of a stochastic differential equation. The process of diffusion is driven by two physical parameters, the relaxation or correlation time τ and the velocity diffusivity coefficient D_v. An extension of the classical Langevin approach by means of a population of τ and D_v is here considered to generate a fractional dynamics. This approach supports the idea that fractional diffusion in complex media results from Gaussian processes with random parameters, whose randomness is due to the medium complexity. A statistical characterization of the complex medium in which the diffusion occurs is realized deriving the distributions of these parameters. Specific populations of τ and D_v lead to particular fractional diffusion processes.

This approach allows for preserving the classical Brownian motion as basis and it is promising to formulate stochastic processes for biological systems that show complex dynamics characterized by fractional diffusion.

A numerical study of this new alternative approach represents the core of the present thesis.

The main features of Brownian dynamics are described in Chapter 1, both for a free particle and for a particle confined by a harmonic potential. In Chapter 2 a short review of some models discussed in literature for fractional diffusion is presented, together with its peculiar features. In Chapter 3 we describe a new approach based on the Langevin equation to generate the fractional kinetics; in this approach superdiffusion is obtained as a generalization of the Langevin equation for a free particle while the subdiffusive case needs the introduction of a confining potential. Some analytical results presented in this

Chapter have been derived by Silvia Vitali during her research period abroad in BCAM, Bilbao, under the supervision of Dr. Gianni Pagnini. In Chapter 4 the numerical results of this approach for the particular case of superdiffusion are showed with an in-depth study of the generated stochastic processes. Finally in the Appendix it is reported the definitions of the fractional derivatives and some useful features of the Mainardi function and the Lévy stable distributions.

Chapter 1

Brownian Dynamics

The Brownian motion was observed for the first time by Robert Brown in 1827 [1]and its first mathematical formulation was provided by Albert Einstein in 1905 [3]. It describes the random motion of particles immersed in a fluid. The latter, thought as a set of an enormous number of microscopic particles characterized by their own thermal motion, represents a *homogenous medium* that stimulates with continuos collisions the particles immersed in it.

The theoretical description of the Brownian motion involves many formulations including phenomenological, probabilistic and microscopic approaches. Here the attention is focused on a mesoscopic description in terms of a stochastic equation of motion: the Langevin Equation.

1.1 Langevin equation

A Brownian particle[1] which moves along a specific direction x is taken into cosideration. The dynamic of this particle is described by the following stochastic equation which is called *Langevin equation*

$$m\frac{d^2x}{dt^2} = -\gamma\frac{dx}{dt} + \Gamma\xi(t)\,, \tag{1.1}$$

where m is the mass of the Brownian particle, γ is the friction coefficient and Γ the noise intensity. The term $\xi(t)$ represents an unknown stochastic force due to the effect of all the particles which constitute the surrounding *medium* and is referred to as "noise source". This force, which is responsible for the fluctuations of the Brownian particle, is countered by the friction term (the first term on the right-side of Eq. (1.1)), generated from the surrounding *medium* as well.

[1]A Brownian particle means a heavy particle immersed in a fluid of light molecules which collide with them in a random way.

The stochastic force, called *Langevin force*, is irregular and unpredictable but it has two main properties which are:

- its ensemble average[2] vanishes: $\langle \xi(t) \rangle = 0$;
- it varies rapidly; the idea is that every collision of the Brownian particle with a single particle of the surrounding fluid is instantaneous and uncorrelated with the successive collisions: $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$.

A stochastic force with these characteristics is defined *White Noise* due to the fact that using the *Wiener-Khintchine* theorem[3] it is possible to see that its spectral density $S(\omega)$ is a constant:

$$S(\omega) = 2 \int_{-\infty}^{+\infty} e^{-i\omega t'} \delta(t') dt' = 2 \, .$$

By means of the stochastic integration of white noise one can prove the Gaussianity of the Langevin force since it results to be a Wiener process which is, indeed, a Gaussian process characterized by:

$$W(t, \tau) = \int_{t}^{t+\tau} \xi(t') dt' \implies dW(t) = \xi(t) dt, \quad \langle dW(dt) \rangle = 0 \quad \langle dW^2(dt) \rangle = dt. \tag{1.2}$$

If we define $v(t) = dx/dt$ the velocity of the Brownian particle, the Langevin equation can be written as a stochastic differential equation:

$$dv(t) = -\frac{\gamma}{m} v(t) dt + \frac{\Gamma}{m} dW(t) \, . \tag{1.3}$$

The Equation (1.3) defines $v(t)$ as a stochastic process. Fixed an initial value $v(t_0) = v_0$, an explicit formal solution for (1.3) can be written as

$$v(t) = v(0) e^{-\gamma(t-t_0)/m} + \frac{1}{m} \int_{t_0}^{t} e^{-\gamma(t-t')/m} dW(t') \, . \tag{1.4}$$

Then if we introduce the velocity diffusivity coefficient D_v and the relaxation time scale τ

$$D_v = \frac{\Gamma^2}{2m^2}; \quad \tau = \frac{m}{\gamma} \, , \tag{1.5}$$

[2]The ensemble may consist of either many particles on the same field or of a series of observations of the same particle. In the first case one must ensure that the distance from one particle to another is so large that they not influence each other. In the second case one must ensure that the time from one observation to another is so long that the system has the time to return to equilibrium.

[3]The Wiener-Khintchine theorem relies the Fourier spectrum of an autocorrelation function to the Fourier spectrum of the corresponding dynamical variable itself. In our case, recalling the autocorrelation function of the noise $C(t) = \int_{-\infty}^{+\infty} \xi(t')\xi(t - t')dt'$, the theorem asserts that $\mathcal{F}\Big[|\xi(t)|^2\Big] = S(\omega) = \mathcal{F}[C]$.

Equation (1.3) becomes

$$dv(t) = -\frac{1}{\tau}v(t)dt + \sqrt{2D_v}dW(t) \tag{1.6}$$

and (1.4) can be written as follows:

$$v(t) = v_0 e^{-(t-t_0)/\tau} + \sqrt{2D_v}\int_{t_0}^{t} e^{-(t-t')/\tau}dW(t')\,. \tag{1.7}$$

1.2 Ornestein-Uhlenbeck process

We now focus the attention on (1.7) which is reported below for convenience

$$v(t) = v_0 e^{-(t-t_0)/\tau} + \sqrt{2D_v}\int_{t_0}^{t} e^{-(t-t')/\tau}dW(t')\,. \tag{1.8}$$

The process described by this equation is called Ornstein-Uhlenbeck (OU) process. It was originally introduced to describe a Brownian particle's velocity, as we did, but nowadays it is also used for many other applications in physics.

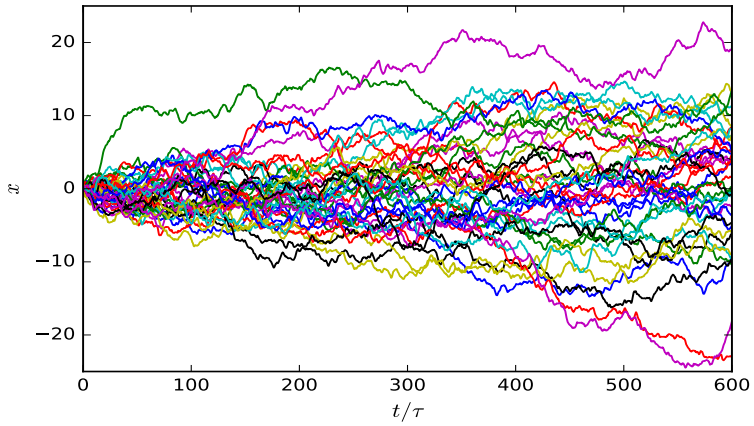


Figure 1.1: Particle trajectories of the Langevin equation.

Since $dW(t)$ is a Gaussian process and because of the linearity of (1.3), $v(t)$ will be a Gaussian process as well and thus, it will be completely defined once found the first two moments. Taking the average of (1.8) and considering that $\langle dW(t)\rangle = 0$, we find

$$\langle v(t)\rangle = v_0 e^{-(t-t_0)/\tau}\,. \tag{1.9}$$

From (1.8) it is also possible to calculate the correlation function of $v(t)$ defined as

$$\begin{aligned} C_v(t_2,t_1) &= \langle v(t_2)v(t_1)\rangle \\ &= \langle v_0^2\rangle e^{-(t_2-t_1)/\tau} + 2D_v \int_{t_0}^{t_2}\int_{t_0}^{t_1} e^{-(t_2-t_2')/\tau} e^{-(t_1-t_1')/\tau} \langle dW(t_2')dW(t_1')\rangle \,. \end{aligned} \tag{1.10}$$

In the previous equation is implied that $\langle v(0)dW(t)\rangle = 0$ at any time; this is because the Langevin force acts as an external force thus, at any time, it is independent from the kinematic properties of the particle.

The only contribution of the integral in (1.10) is for $t_2' = t_1'$ since the Wiener process has, except for this case, zero correlation function. Thus we have

$$\begin{aligned} C_v(t_2,t_1) &= \langle v_0^2\rangle e^{-(t_2-t_1)/\tau} + 2D_v \int_0^{\min\{t_2,t_1\}} e^{-(t_2+t_1-2t_1')/\tau} dt_1' \\ &= (\langle v_0^2\rangle - D_v\tau) e^{-(t_2+t_1-2t_0)/\tau} + D_v\tau e^{-(|t_2-t_1|)/\tau} \,. \end{aligned} \tag{1.11}$$

The correlation function in (1.11) allows to get directly the second moment of the velocity $v(t)$

$$\sigma_v^2(t) = \big\langle (v - \langle v(t)\rangle)^2 \big\rangle(t) = D_v\tau\big(1 - e^{-2(t-t_0)/\tau}\big) \,. \tag{1.12}$$

After an initial transient of the order of a few relaxation time scale units, the σ_v^2-value reaches a long-time equilibrium. For the stationary state we thus have

$$\sigma_{v,eq}^2 = D_v\tau \quad C_{v,eq}(|t_2-t_1|) = R(t=|t_2-t_1|) = \sigma_{v,eq} e^{-t/\tau} \,. \tag{1.13}$$

The velocity described by the OU process is thus a Gaussian stochastic process that undergoes the following distribution

$$G_v(v,t) = \frac{1}{\sqrt{2\pi\sigma_v^2(t)}} \exp\Big\{ - \frac{(v - \langle v(t)\rangle)^2}{2\sigma_v^2(t)} \Big\} \,, \tag{1.14}$$

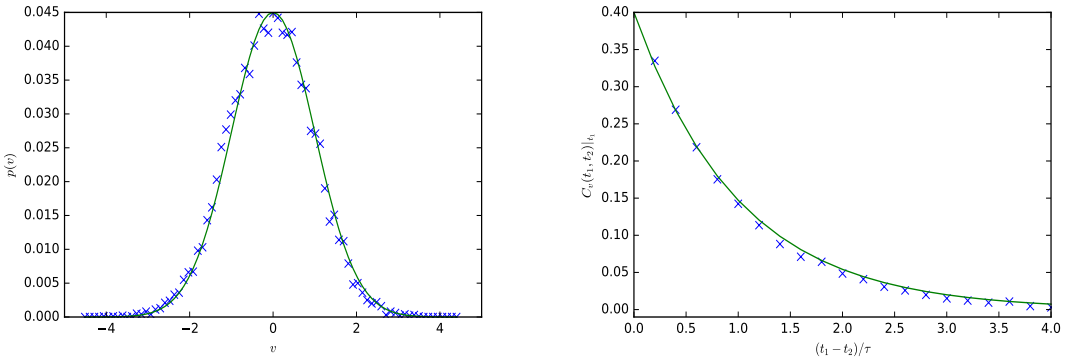
where the mean value and the variance is respectively defined by (1.9) and (1.12). The stationary, equilibrium distribution is attained for $t \to +\infty$ and it becomes effective in the time range $t \gg \tau$:

$$G_{v,eq}(v) = \frac{1}{\sqrt{2\pi D_v\tau}} \exp\Big\{ - \frac{v^2}{2D_v\tau} \Big\} \,. \tag{1.15}$$

For the variance, recalling Eq. (1.13), we have:

$$\sigma_{v,eq}^2 = D_v\tau_c = \frac{\Gamma^2}{2m\gamma} \,, \tag{1.16}$$

while for the mean we can say that, at the equilibrium, if there are no external forcing it is zero.



(a) *Velocity pdf.* (b) *Velocity correlation function.*

Figure 1.2: OU process velocity in stationary state: pdf and correlation function.

It is worth noting that the velocity distribution of any particle which is in thermodynamic equilibrium with its environment is the well-known Maxwell-Boltzmann velocity distribution:

$$p_{eq}(v) = \sqrt{\frac{m}{2\pi kT}} \exp\Big\{ -\frac{mv^2}{2kT} \Big\} \tag{1.17}$$

with k and T the Boltzmann constant and temperature respectively. Comparing (1.17) with (1.15) it is possible to find a particular case for the relation (1.16) that shows clearly how friction and velocity diffusivity are related to each other through:

$$D_v \tau_c = \frac{kT}{m} \iff kT = \frac{\Gamma^2}{2\gamma} \,. \tag{1.18}$$

1.3 Taylor theorem

The Langevin equation can be also solved for the particle displacement, which is given by

$$x(t) = x(0) + \int_{t_0}^{t} v(t')dt' \,.$$

In fact, what we are interested in is the mean square displacement and it can be associated with the velocity correlation function, noting that

$$\begin{aligned} \sigma_x^2(t) &= \langle (x(t) - x_0)^2 \rangle = \Big\langle \Big[\int_{t_0}^{t} v(t')dt' \Big]^2 \Big\rangle \\ &= \Big\langle \int_{t_0}^{t} v(t')dt' \int_{t_0}^{t} v(t'')dt'' \Big\rangle = \int_{t_0}^{t} \int_{t_0}^{t} \langle v(t')v(t'') \rangle dt'dt'' \,. \end{aligned} \tag{1.19}$$

It is quite easy to solve the integral above when the system is in its stationary state:

$$\sigma_x^2(t) = \int_{t_0}^{t}\int_{t_0}^{t} C_v(t', t'')dt'dt'' = 2\int_{t_0}^{t}(t-s)R(s)ds\,, \tag{1.20}$$

or equivalently

$$\frac{d\sigma_x^2(t)}{dt^2} = 2\int_{t_0}^{t} R(s)ds\,. \tag{1.21}$$

These equations was first studied by Taylor, who formulated this theorem for the normal diffusion process:

Theorem 1. *[32]*
Given the stationary correlation function $R(t)$ let us define the correlation time scale:

$$\tau = \int_0^{\infty} \frac{R(s)}{R(0)}ds, \quad R(0) = \sigma_{v,eq}^2\,, \tag{1.22}$$

then the following crucial assumption:

$$0 \neq \tau < +\infty \tag{1.23}$$

always determines the emergence of normal diffusion in the long-time regime:

$$\sigma_x^2(t) = 2D_x t; \quad D_x := \lim_{t\to+\infty} \frac{d\sigma_x^2}{dt^2}(t) \quad t \gg \tau\,, \tag{1.24}$$

independently from the micro-dynamics.

Back to the OU process, solving Eq. (1.20) considering Eq. (1.13), we find out that:

$$\sigma_x^2(t) = 2D_v\tau^2(t-t_0) - 2D_v\tau^3(1-e^{-(t-t_0)/\tau})\,. \tag{1.25}$$

From (1.25) we can see that the mean square displacement presents two different trends, depending on the time range:

$$\langle (x(t)-x_0)^2 \rangle = \begin{cases} 2D_v\tau t^2 & \text{se } t \ll \tau \\ 2D_v\tau^2 t & \text{se } t \gg \tau\,. \end{cases} \tag{1.26}$$

Equation (1.26) shows that for time much longer than the relaxation time the mean square displacement grows linearly with time while, for the initial phase, it has indeed a parabolic form. Once reached the stationary equilibrium, represented by the linear trend of $\sigma_x^2(t)$, we can define a diffusivity coefficient for the displacement given by $D_x = D_v\tau^2$. If we put it in the Eq. (1.16) we find out an important relation known as *Einstein-Smoluchowski relation*:

$$D_x = D_v\tau^2 = \frac{\Gamma^2}{2\gamma^2} = \frac{kT}{\gamma}\,. \tag{1.27}$$

1.4 Brownian motion in a harmonic potential

Now a Brownian particle which diffuses under the influence of an external harmonic potential $V(x) = kx^2/2$, with the corresponding force acting on the particle $F_h = -kx$ is considered. The Langevin equation in this case is:

$$\begin{cases} \dfrac{dx}{dt}(t) = v(t) \\ \dfrac{dv}{dt}(t) = -\dfrac{1}{\tau}v(t) - \omega_0^2 x(t) + \sqrt{2D_v}\xi(t) \end{cases} \tag{1.28}$$

where $\omega_0^2 = k/m$. After application of the Fourier transform:

$$\begin{cases} -i\omega x(\omega) = v(\omega) \\ -i\omega v(\omega) = \dfrac{1}{\tau}v(\omega) - \omega_0^2 x(\omega) + \sqrt{2D_v}\xi(\omega) \end{cases} \tag{1.29}$$

we can solve the obtained linear system for $x(\omega)$, in terms of the Langevin force

$$x(\omega) = \sqrt{2D_v}\frac{\xi(\omega)}{\omega_0^2 - \omega^2 - \frac{1}{\tau}i\omega}\,. \tag{1.30}$$

The spectral density $S_x(\omega)$ is proportional to $|x(\omega)|^2$ so we have

$$S_x(\omega) = 2D_v\frac{S_\xi(\omega)}{|\omega_0^2 - \omega^2 - \frac{1}{\tau}i\omega|^2} = 2D_v\frac{2\Gamma}{((\omega_0^2 - \omega^2)^2 + \frac{1}{\tau^2}\omega^2)}\,, \tag{1.31}$$

from which, thanks to the Wiener-Khintchine theorem the correlation function can be found

$$C_x = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{-i\omega t}S_x(\omega)d\omega\,. \tag{1.32}$$

The integral can be calculated in the complex plane, taking the residues at the poles located at

$$\omega_0^2 - \omega^2 = \pm\frac{1}{\tau^2}i\omega \implies \omega = \pm i\frac{1}{2\tau} \pm \sqrt{\omega_0^2 - \frac{1}{4\tau^2}} \implies \omega = \pm i\frac{1}{2\tau} \pm \omega_1\,.$$

Working out the residues it can be found

$$C_x(t) = \frac{D_v\tau}{\omega_0^2}e^{-(t-t_0)/2\tau}\Big\{\cos\omega_1 t + \frac{1}{2\tau\omega_1}\sin\omega_1 t\Big\}\,. \tag{1.33}$$

With an analogous method we can find the spectral density for the velocity correlation, which is correlated to the displacement one through

$$S_v(\omega) = \omega^2 S_x(\omega)\,. \tag{1.34}$$

We notice that for $t = 0$, $C_x(0) = \langle x_0^2\rangle = D_v\tau/\omega_0^2 = kT/m\omega_0^2$ which just identifies the equipartition of the energy.

1.5 Relation to Fokker-Planck equation

The Fokker-Planck equation, which can be seen in the general case as an approximation of a Master equation, is also known as "Smoluchowski equation", "generalized diffusion equation" or "second Kolmogorov equation" and it is given by

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}A(x)P(x,t) + \frac{1}{2}\frac{\partial^2}{\partial x^2}B(x)P(x,t)\,. \tag{1.35}$$

where the coefficients $A(x)$ and $B(x)$ can be any real function with the only restriction $B(x) > 0$. The first term on the right-hand represents the "drift term" while the second represents the "fluctuation/diffusion term". The two coefficients can be easily found for every stochastic process with a minimum knowledge about the underlying mechanism. Suppose x to be a Markov process and then take a short time Δt, so short that x cannot vary too much, but large enough for the Markov assumption[4] to be applied and now compute the average along Δt of Δx and $(\Delta x)^2$. It is possible to demonstrate that

$$\frac{\langle \Delta x \rangle}{\Delta t} = A(x), \qquad \frac{\langle (\Delta x)^2 \rangle}{\Delta t} = B(x)\,. \tag{1.36}$$

The Fokker-Planck equation describing a Wiener process doesn't have the term with the derivative of the first order so it appears as a diffusion equation; in fact, it is the diffusion equation for the Brownian particle in the fluid

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}\,. \tag{1.37}$$

The foundamental solution of Equation (1.37), is the Gaussian

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}}\exp\Big\{-\frac{x^2}{4Dt}\Big\}\,, \tag{1.38}$$

which has zero mean and a width that evolves linearly with the square root of time, according to $\sqrt{\langle x^2(t)\rangle} = \sqrt{2Dt}$.
The Fokker-Planck equation describing an OU process in the phase space is given by:

$$\frac{\partial P(v,x,t)}{\partial t} = D_v\frac{\partial^2 P(v,x,t)}{\partial v^2} - \frac{1}{\tau}\frac{\partial v P(v,x,t)}{\partial v} - v\frac{\partial P(v,x,t)}{\partial x}\,. \tag{1.39}$$

Although one might think that the Langevin equation, (1.3) and the Fokker-Planck equation (1.39) are equivalent, in fact they are not. The latter fully defines the stochastic process, while the former cannot go beyond the first two moments of the stochastic process described because the higher moments from the Langevin force are unknown.
Indeed, in the specific case of Brownian motion, the two equations mentioned before coincide since we are dealing with a Gaussian process, which is totally described by its first two moments.

[4]For a dynamical system the Markov assumption asserts that given the present state, all following states are independent of all past states.

Chapter 2

Fractional Dynamics

2.1 Main features of fractional diffusion

The main results of Brownian motion theory are the mean square displacement scaling linearly with time and a Gaussian normal distribution as probability density function. We deduced these characteristics in Chapter 1 through a Langevin approach, but they are consistent across many mathematical descriptions and many experiments have verified these features.

However standard diffusion is not universal. In literature there are numerous experimental measurements [19, 4, 7, 15, 16, 31, 34] showing non linear diffusion. It is used to refer to these phenomena with the term *anomalous* diffusion because of the anomalous scaling of the position variance manifested in power laws: in particular if the exponent is less the unity we have *subdiffusive* processes instead, if the exponent is greater than unity we have *superdiffusive* processes

$$\langle x^2(t)\rangle \sim K_\phi t^\phi \quad \text{with} \quad \phi \neq 1\,. \tag{2.1}$$

Actually the concept of anomalous dynamics encloses many properties such as stretched exponential, colored noises, non Gaussian pdfs and a long-range spatial or temporal correlations. In recent years a great deal of progress has been made in extending the different models for diffusion to incorporate this anomalous diffusion [5]. The tools of fractional calculus have proven very useful [29] in these developments, linking together many mathematical models like fractional constitutive laws, continuous time random walks, fractional Langevin equations and fractional Brownian motions. So that anomalous diffusion is also referred to as *fractional* diffusion.

Space-Time fractional diffusion was originally introduced to study chaotic dynamics where a non-local and/or non-linear relationship is needed. In the fractional calculus approach the idea is to maintain a linear relationship while introducing a non-local dependence by means of integral operators with inverse power-law kernel. Non linearity

can be considered in time (*time fractional diffusion* or in space (*space fractional diffusion*) or both (*space-time fractional diffusion*). Under the physical point of view, when there is no separation of timescale between the microscopic and the macroscopic level of the process the randomness of the microscopic level is transmitted to the macroscopic level and the correct description of the macroscopic dynamics has to be in terms of the fractional calculus. Fractional kinetics strongly differs form the classical one because some moments of the pdf of particle displacement can be infinite and the fluctuations from the equilibrium state have a broad distribution of relaxation times.

The *space-time fractional diffusion* equation is defined by [9]:

$$ {}_{\mathrm{t}}\mathrm{D}^{\beta}_{*} P(x;t) = {}_{x}\mathrm{D}^{\nu}_{\theta} P(x;t), \quad -\infty < x < +\infty, \quad t \geq 0\,, \tag{2.2} $$

with $P(x;0) = P_0(x)$ and $P(\pm\infty;t) = 0$. ${}_{\mathrm{t}}\mathrm{D}^{\beta}_{*}$ is the *Caputo time-fractional derivative* [B] of order β while ${}_{x}\mathrm{D}^{\alpha}_{\theta}$ is the *Riesz-Feller space fractional derivative* [B] of order ν and symmetry parameter θ. The real parameters α, β and θ are restricted as follows:

$$ 0 < \nu \leq 2, \quad |\theta| \leq \min\{\nu, 2-\nu\}, \quad 0 < \beta \leq 1 \quad \text{or} \quad 0 < \beta \leq \nu \leq 2\,. \tag{2.3} $$

A general solution for Eq. (2.2) can be represented by:

$$ P(x;t) = \int_{-\infty}^{+\infty} K^{\theta}_{\nu,\beta}(x-x';t) P_0(t) dx'\,, \tag{2.4} $$

where $K^{\theta}_{\nu,\beta}(x;t)$ is the Green function or fundamental solution which has been expressed by the Mellin-Barnes integral representation as well as in terms of H-Fox function [9, 12]. Particular cases of the (2.2) are the space fractional diffusion when $\beta = 1$, time fractional diffusion when $\nu = 2$ and standard diffusion when $\beta = 1$ and $\nu = 2$. Physically speaking the first one is related to the long range memory (non Markovian processes) while the second one is referred to non Gaussian particle displacement pdf, thus non locality. Essentially we can see (2.2) as a Master equation and its solution as a pdf of the underlying stochastic process. In the following sections we are going to present some different approaches which allow to get anomalous diffusion stochastic processes.

2.2 Continuos time random walk

The *Continuos time random walk* (CTRW) model was introduced by Montroll and Weiss [21] and can be viewed as a direct generalization of the *Random walk* also known as *drunkard's walk*. In the standard random walk the step length is a fixed Δx and the steps occur at discrete times separated by a fixed time interval Δt.

The CTRW chooses a waiting time from a waiting time probability density $\phi(\Delta t)$ before each step and the step length is chosen from a step length probability density $\psi(\Delta x)$. Physically, such waiting times reflect the existence of deep traps in the system

which subsequently immobilize the diffusing particle. An important feature of this model is also its renewal character: after each jump, values of the new pair of random variable are fully independent of their previous values. It is further assumed that the waiting times and step lengths are independent of each other so that:

$$\Psi(x - x', t - t') = \psi(x - x')\phi(t - t') \,. \tag{2.5}$$

It is useful to define the survival probability

$$\Phi(t) = 1 - \int_0^t \phi(t')dt' = \int_t^\infty \phi(t')dt' \,, \tag{2.6}$$

which is the probability that the walker does not step during the time interval t.

The fundamental quantity to calculate in this model is the conditional probability density $p(x; t|x_0, t_0)$ that a walker starting from position x_0 at time t_0 , is at position x at time t. This can be obtained from the *Master equation* of the CTRWs:

$$p(x; t|x_0, t_0) = \Phi(t)\delta_{x,x_0} + \int_{t_0}^t \phi(t - t') \int_{-\infty}^{+\infty} \psi(x - x')p(x'; t'|x_0, t_0)dx'dt' \,. \tag{2.7}$$

The first term of Eq. (2.7) represents the persistence of the walker at the initial position and the second term considers walkers that were at other positions x' at time t' but then stepped to x at time t after waiting a time $t - t'$.

In this model it is possible to distinguish sub- and super- diffusion depending on the different choices for the waiting time and step length density probability. In particular the attention is focused on the average of the waiting time $\langle \Delta t \rangle$ and on the variance of jump length $\langle \Delta x^2 \rangle$. If these moments are both finite we obtain classical diffusion. If we have a finite $\langle \Delta x^2 \rangle$ and the mean waiting time is infinite we obtain subdiffusion. Finally if the step length variance diverges we have superdifusion. In particular, if the waiting time pdf has finite moments the process obtained is called *Lévy flights*; the trajectories of the *Lévy flights* are fractal. There is also studies considering the combination of a diverging characteristic waiting time with a Lévy stable distribution of step lengths. The divergence of $\langle \Delta x^2 \rangle$ which has no physical meaning can be rectified by a cutoff in the jump length pdf.

We note that superdiffusion cannot be achieved within the approach of a generalized waiting time concept. Another possible approach to obtain the superdiffusion is to introduce a coupling between jump lengths and waiting times in the subdifussive framework; this case is referred to as *Lévy walks*. To introduce a coupling between step lengths and waiting times is equivalent to set a constraint in the velocity and so that it corresponds to truncate the velocity pdf.

Note that apart from the finiteness of moments $\langle \Delta t \rangle$ and $\langle \Delta x^2 \rangle$, the details of the related pdfs are irrelevant for the diffusive properties of the CTRW process.

In the subdiffusive case the evolution of the displacement probability function is described by a time fractional diffusion equation:

$$\frac{\partial P(x;t)}{\partial t} = {}_0\mathrm{D}_t^{1-\alpha} K_\alpha \frac{\partial^2 P(x;t)}{\partial x^2}\,, \tag{2.8}$$

where ${}_0\mathrm{D}_t^{1-\nu}$ is the Riemann-Liouville fractional derivative. The foundamental solution of Eq. (2.8) shows an asymptotic behavior corresponding to a stretched Gaussian. Comparing Eq. (2.8) with the dynamical equation for the fBM reported below in (2.10) we can notice that the latter, conversely to the former, is perfectly local in time. This characteristic represents the main difference between this two model. CTRW leads to highly non-local processes with long correlations in space and/or time; fBM and generalized Langevin equation (GLE), on the macroscopic level, are local in space and time and carry time- or space- dependent coefficients.

As far as the superdiffusive case is concerned it is possible to define a dynamical equation for the Lévy flights which we can referred to as Lévy fractional diffusion equation:

$$\frac{\partial P(x;t)}{\partial t} = K^\nu \frac{\partial^\nu P(x;t)}{\partial |x|^\nu}\,. \tag{2.9}$$

It defines a Lévy stable law and furthermore it highlights the strongly non-local character of Lévy flights. For the specific case of the Lévy walks building an analytic equation essentially is more difficult because of what we said before about the truncation of the pdf.

2.3 Fractional Brownian motion

Both in the presence and in the absence of external potential the *fractional Brownian motion* (fBM) represents, together with the already described CTRW, one of the major stochastic model for the description of the anomalous diffusion processes. There is a vaste literature on fBM, starting with Mandelbrot and Van Ness [14] and it comes from one of the easiest ways to model anomalous diffusion: replacing the constant diffusivity with a time dependent diffusivity $D(t) = 2Ht^{(2H-1)}D$. In this case the evolution equation for the probability density function becomes:

$$\frac{\partial P}{\partial t}(x,t) = 2Ht^{(2H-1)} D \frac{\partial^2 P}{\partial x^2} D(t)\,. \tag{2.10}$$

The fBM is a stochastic process distinguished by the fact that it is the only self-simialrity Gaussian process with stationary increments, as a metter of fact if we let $B_H(t)$ denote a fBM stochastic process with Hurst exponent $H \in [0,1]$ then three properties of particular note are:

- correlations
$$E\big(B_H(t)B_H(t')\big) = \frac{1}{2}\big(|t|^{2H} + |t'|^{2H} - |t-t'|^{2H}\big),$$
- Self-similarity
$$B^B(at) = |a|^H B^H(t),$$
- Realizations $x_B(t)$ of the process are continuous but nowhere differentiable.

The fBm can be defined by means of a stochastic integral:

$$x_B(t) = \frac{1}{\Gamma\big((1-2H)/2\big)}\Big[\int_0^t (t-t')^{(2H-1)/2} dB(t') + \int_{-\infty}^0 \big(t-t')^{(2H-1)/2} - (-t')^{(2H-1)/2}\big) dB(t')\,. \tag{2.11}$$

The probability density function for the fBm is given by the stretched Gaussian

$$P(x,t) = \frac{1}{\sqrt{4\pi K_{2H} t^{2H}}} \exp\Big(-\frac{x^2}{4K_{2H}t^{2H}}\Big)\,, \tag{2.12}$$

and the position autocorrelation is

$$\langle x_B(t) x_B(t')\rangle = K_{2H}\big(t^{2H} + t'^{2H} - |t-t'|^{2H}\big)\,. \tag{2.13}$$

This model describes processes with an antipersistent behavior if $0 < 2H < 1$ and persisten if $1 < 2H \leq 2$.

2.4 Fractional Langevin equation

The fBm can also be defined by means of more intuitive representation uses the *fractional Langevin equation* (fLE):

$$m\frac{d^2x_B}{dt^2} = -m_0 \mathrm{D}_t^{2H} x_B(t) + \xi_{fGn}(t) \quad , \tag{2.14}$$

where $B(t)$ is ordinary Brownian motion and $\xi_{fGn}(t)$ is the fractional Gaussian noise which has a standard normal distribution for any $t > 0$ but it is power-law correlated. Note that the fLE represents a particular case of the generalized Langevin equation (GLE) which is reported below:

$$m\frac{d^2x(t)}{dt^2} = -\gamma \int_0^t K(t-t')\frac{dx}{dt'}dt' + \xi(t)\,, \tag{2.15}$$

where $\xi(t)$ is a non-white noise and $K(t)$ is a memory kernel which satisfied the *Fluctuation-Dissipation Theorem*: $\langle \xi(t)\xi(t')\rangle = k_B T K(t-t')$. The fLE is obtained in the specific case of $\xi(t)$ equal to a fractional Gaussian noise.

2.5 Generalized grey Brownian motion

The *generalized grey Brownian motion* (ggBM) [23, 22, 20] is a class of stochastic processes defined by:

$$X_{\beta,H} = \sqrt{\Lambda_\beta} X_H(t)\,, \tag{2.16}$$

where the random variable Λ_β is defined as a Mainardi function $M_\beta(\lambda)$ with $\lambda \geq 0$ and $0 < \beta \leq 1$. The stochastic process X_H is a Gaussian process with a variance scaling with t^{2H} and it is generally considered to be a fBM. This model involves the *grey Brownian motion* (gBM) for $\beta = 2H$, the fBM for $\beta = 1$ and the Brownian motion (BM) for $\beta = 2H = 1$.

The evolution equation for the pdf of the ggBM can be expressed in term of the *Erdély-Kober* $D_\eta^{\epsilon,\mu}$ fractional derivative with respect to t in the following way [25]:

$$\frac{\partial P}{\partial t} = \frac{\nu}{\beta} t^{\nu-1} D^{\beta-1,1-\beta}_{\nu/\beta} \frac{\partial^2 P}{\partial x^2}\,, \tag{2.17}$$

so that we con also referred to this process as *Erdély-Kober fractional diffusion*. The Green function for Eq. (2.17) corresponds to:

$$P(x;t) = \frac{1}{2t^H} M_{\beta/2}\Big(\frac{|x|}{t^H}\Big)\,. \tag{2.18}$$

Physically these processes can be thought as a population of particles diffusing according to a Gaussian process X_H in a complex random medium. This medium has properties that are independent from the particles and it has a randomness described by a characteristic quantity with distribution depends on β. This parameter has thus to role of driving the randomness of the medium.

The same approach has been used [26] to derive a stochastic process whose one-point one-time pdf is the solution of the symmetric space-time fractional diffusion, which occurs when in Eq. (2.2) $\theta = 0$. It can be defined(ref) as:

$$X_{\nu,\beta}(t) = \sqrt{\Lambda_{\nu/2,\beta}} G_{2\beta/\nu}(t), \quad 0 < \beta \leq 1, \quad 0 < \nu \leq 2\,, \tag{2.19}$$

where $G_{2\beta/\nu}(t)$ is a H-SSSI [1] Gaussian process with power law variance $t^{2\beta/\nu}$ and $\Lambda_{\nu/2,\beta}$ is an independent constant non-negative random variable distributed according to the pdf $K^{-\nu/2}_{\nu/2,\beta}(\lambda), \quad \lambda \geq 0$. The stochastic process described in (2.19) generalizes Gaussian processes and it is uniquely determined by the mean and the autocovariance structure.

[1] A stochastic process $X(t)$, $t \geq 0$ with values in R is a *Hurst Self-Similar with stationary Increments*(H-SSSI) process if:

(i) it is a self-similar process, $X(at) = a^H X(t)$;

(ii) it has stationary increments, $X(t+t') - X(t)$ is invariant under time shift transformation.

In comparison with the ggBM it involves also stochastic processes fractional in space but on the other hand it doesn't provide all the time fractional processes described by the ggBM.

Going on we will see that this approach has some characteristics in common with the approach we will deal with in Chapter 3 and 4. In particular the idea is essentially the same but the way to obtain the Gaussian process with an anomalous scaling is totally different. This difference will allow us to treat a larger variety of processes.

Chapter 3

An Alternative Approach

The Langevin equation, as we saw in Chapter 1, is driven by two parameters: the friction and the noise amplitude. Here is proposed[1] a statistical characterization of the complex medium in which the diffusion occurs by randomizing these parameters and their distributions are derived.

We consider parameters modulation in the Langevin equation to generate a fractional kinetics. Taking into account a free particle in a viscous medium it is possible to describe anomalous super-diffusive regimes, while introducing a confining term in the equation (Langevin harmonic oscillator) but maintaining the same parameter modulation, we can describe subdiffusive regimes.

This approach supports the idea that fractional diffusion in complex media results from Gaussian processes with random parameters, whose randomness is due to the medium complexity.

This model is promising to formulate stochastic processes for biological systems that show complex dynamics characterized by anomalous diffusion and it allows for preserving the classical Brownian motion as basis.

3.1 Sub- and super-diffusion

We showed in Chapter 1 that, when the assumption (1.23) of the Taylor theorem about the finite and non zero value of τ is still valid, there is a well-defined correlation time scale τ and the emergence of a normal diffusion scaling ($\langle x^2 \rangle \sim t$) in the long-time limit ($t \gg \tau$). As a consequence, the emergence of anomalous diffusion is strictly connected to the failure of this assumption.

In particular when the assumption of finite and non-zero τ fails, we have two cases:

[1] **Some analytical results presented in this Chapter have been derived by Silvia Vitali during her research period abroad in BCAM, Bilbao, under the supervision of Dr. Gianni Pagnini.**

- Super-diffusion:
$$\int_0^\infty \frac{R(s)}{R(0)} ds = +\infty \ , \tag{3.1}$$
and we have: $\langle x^2 \rangle \sim t^\alpha$ with $\alpha > 1$ or $\langle x^2 \rangle = \infty$

- Sub-diffusion:
$$\int_0^\infty \frac{R(s)}{R(0)} ds = 0 \, , \tag{3.2}$$
and, thus, $\langle x^2 \rangle \sim t^\alpha$ with $\alpha < 1$. This case occurs when there is anti-correlation, i.e., there exist time lags t such that $R(t) < 0$ (e.g., the anti-persistent fBM with $H < 0.5$).

3.2 Anomalous diffusion by randomization of the timescale and diffusivity parameters

In the following we use the fundamental results of the Langevin description to derive a model for anomalous diffusion. The basic idea is that the observed anomalous diffusion emerges as a linear superposition of independent contributions, each contribution being given by a single realization of the process. The superposition is driven by the randomness of some parameters and these parameters are here treated as independent random variables with a given pdf.

We assume that the randomness lies in the parameters D_v and/or τ or, equivalently, in the parameters γ and/or Γ. Each chosen parameter is statistically independent from the other ones.

Thus, the following pdfs are given:

$$h(D_v) \ ; \quad b(\tau) \ ; \quad f(\gamma) \ ; \quad g(\Gamma) \, . \tag{3.3}$$

Considering Eq. (1.5), the pdfs $h()$ and $g()$ are related to each other, and so are the pdfs $b()$ and $f()$.

Starting from the basic formulas of the considered stochastic process, the parameter pdf driving the linear superposition is here chosen in such a way to determine the emergence of global (effective) statistical features in agreement with fractional anomalous diffusion. The basic formulas that we exploit in the proposed extension of the classical Langevin approach are the following:

- Eq. (1.13) for the velocity correlation function;
- Eqs. (1.20) and (1.21) for the variance of the position in the stationary, equilibrium state;

- Eqs. (1.14) and (1.15) for the velocity pdf (general and stationary cases, respectively);
- Eqs. (1.18) and (1.27) for the relationships among velocity and position diffusivities, parameters of the OU model (friction and noise intensity) and equilibrium statistics $\sigma^2_{v,eq}$ (e.g., kT in the Maxwell-Boltzmann equilibrium distribution).

Then, we impose the emergence of the following global properties:

(i) correlation function with a asymptotic power-law decay;

(ii) anomalous diffusion in the position variance;

(iii) pdf $P(x;t)$ compatible with fractional diffusion.

First of all let us define a stochastic variable which is the product of the gaussian variable x_ϕ and an appropriate power of a random variable Λ not dependent on time:

$$x = \sqrt{\Lambda} v_\phi \,, \tag{3.4}$$

velocity changes as well:

$$v = \sqrt{\Lambda} v_\phi \,. \tag{3.5}$$

The classical Langevin equation then becomes:

$$\begin{cases} d\sqrt{\Lambda} x_\phi(t) = \sqrt{\Lambda} v_\phi(t) dt \\ d\sqrt{\Lambda} x_\phi(t) = -\dfrac{1}{\tau}\sqrt{\Lambda} v_\phi(t) dt + \sqrt{2\Lambda D_v} dW(t) \end{cases} \tag{3.6}$$

and $D_V = \Lambda D_v$ is the new random velocity diffusivity coefficient (hereafter we will refer to D_v in the case of non random diffusivity and to D_V in the case of random diffusivity).

Since we assume that τ, D_V are independent parameters and thanks to the possibility to factorize out the parameter $\sqrt{\Lambda}$ in Eq. (3.6), it is possible to consider the randomization of the timescale and of the diffusivity in two separate steps.

3.3 Thermal equilibrium condition

We already remembered in Section 3.1 that the emergence of fractional diffusion is strictly related to the stationary characteristics of the system. An asymptotic power-law behavior for the correlation function is a typical condition violating the assumption of the Taylor Theorem. Let us first rewrite the velocity correlation function of the single

OU process, as given by Eq. (1.11), making the variable dependence more explicit and avoiding the average over the initial velocities:

$$\langle v(t_1)v(t_2)|v_0, D_{_V}, \tau\rangle_\xi = \left(v_0^2 - D_{_V}\tau\right) e^{-(t_1+t_2-2t_0)/\tau} + D_{_V}\tau e^{-|t_1-t_2|/\tau} \,. \tag{3.7}$$

The average over the noise is now conditioned by the random realization of the parameters. Notice that, in the single OU process, the equilibrium condition is associated with the relationship (1.16): $\sigma^2_{v,eq} = \langle v_0^2\rangle_{eq} = D_v\tau$. For the single OU process, this relationship follows by the equilibrium condition given by the Gaussian distribution of Eq. (1.15), which is reached by the OU process in the long-time limit $t \gg \tau$. In this extended model the Gaussian with Eq. (1.15) is no longer the equilibrium pdf for the velocity so that Eq. (1.16) is not valid in general.

Then, even if the equilibrium of the single OU process fails, let us assume that, even in the extended global equilibrium condition, the initial velocity distribution depends on τ: $v_0 = F(\tau, ...)$. Let us now apply the averaging over the random parameters (D_V, τ) and over the initial velocity v_0 to Eq. (3.7):

$$\begin{aligned} &\langle v(t_1)v(t_2)\rangle := \langle\langle v(t_1)v(t_2)|v_0, D_{_V}, \tau\rangle_\xi\rangle_{v_0,D_{_V},\tau} \\ &= \langle\left(v_0^2 - D_{_V}\tau\right) e^{-(t_1+t_2-2t_0)/\tau}\rangle_{v_0,D_{_V},\tau} + \langle D_{_V}\tau e^{-|t_1-t_2|/\tau}\rangle_{v_0,D_{_V},\tau} \,. \end{aligned} \tag{3.8}$$

In order to get the global equilibrium condition, we must put to zero the first, non-stationary, term:

$$\langle v_0^2(\tau) e^{-(t_1+t_2-2t_0)/\tau}\rangle_\tau = \langle D_{_V}\rangle_{D_{_V}} \langle \tau e^{-(t_1+t_2-2t_0)/\tau}\rangle_\tau \,, \tag{3.9}$$

where the dependence of v_0 on τ has been taken into account. This is the equality of two integrals and, thus, the choices on the integrand functions are infinite. However, the most simple and natural choice is given by the following one:

$$v_0^2 = D_{_V}\tau \;; \quad \langle v_0^2\rangle = v^2_{0,eq} = \langle D_{_V}\rangle\langle\tau\rangle \,, \tag{3.10}$$

where the equilibrium assumption on the initial velocity distribution has been taken into account: $\langle v_0^2\rangle_{eq} = v^2_{eq}$.

When stationarity is imposed we can write the following expression for the stationary correlation function:

$$\begin{aligned} R(t) &= \langle v(t_0+t)v(t_0)\rangle = \langle D_{_V}\rangle \left\langle \tau e^{-t/\tau}\right\rangle \\ &= \int_0^\infty dD_{_V} D_{_V} f(D_{_V}) \cdot \int_0^\infty d\tau'\tau' e^{-t/\tau'} \; g(\tau') \,. \end{aligned} \tag{3.11}$$

As a consequence of the fundamental relationship between diffusion of x, $\sigma_x^2(t)$, and velocity correlation function we must guess a suitable choice for $R(t)$ in order to get

anomalous diffusion. This implies to construct suitable distributions for the two random parameters τ and D_V.

Referring at Eqs. (3.1) and (3.2) we saw in particular that in this approach the most general condition leading to the subdiffusive case is that $\int_0^\infty R(t)dt = 0$. This is satisfied if the velocity correlation function $R(t)$ shows an oscillating behavior. This feature cannot be obtained in the free particle case, because the exponential suppression and the distribution function of the timescale present in the correlation function, obtained in Eq. (3.11), are both positively defined. We then expect that to describe subdiffusive processes through the introduction of a further oscillating potential, generalizing the results obtained in the fourth section of Chapter 1.

For the sake of simplicity in the present work we will deal only with the superdiffusive case which can be treated using a free particle model but we highlight that the model for the subdiffusivity is completely defined as well and for more details we remand to the article in press.

3.4 A suitable distribution for τ

Any choice of correlation function and distribution for the parameters of the dynamics should satisfy the following global properties:

- the scaling of the position variance in the long time limit is a power fraction of time;
- the position variance at time zero is zero;
- the scaling of the correlation function in the long time limit should be a power law, with exponent $-\alpha = -(2-\phi)$, with $0 < \alpha < 1$ or $1 < \alpha < 2$ depending if we are describing super or sub diffusive processes respectively;
- the correlation function at time zero is $R(0) = c$, with $c = \sigma^2_{v,eq.}$ finite positive number, which imply that $b(\tau)$, as well as $h(D_V)$, must have finite mean in order to describe a finite energy system;
- the distribution functions of the parameters, $b(\tau)$ and $h(D_V)$, are normalized to 1.

In principle there exists an infinite number of distribution functions $b(\tau)$ that satisfy these conditions, here we propose a suitable function with all the required properties as reference example.

Let's consider a distribution of time scales of the kind:

$$b(\tau) = \frac{\alpha}{\Gamma(1/\alpha)} \frac{1}{\tau} L_\alpha^{-\alpha}\left(\frac{\tau}{\tau_*}\right), \tag{3.12}$$

where $L_\alpha^{-\alpha}(z)$ is the extremal Lévy density, with $0 < \alpha < 1$ and $\tau_* = (\langle\tau\rangle\frac{\Gamma(1/\alpha)}{\alpha})$. The distribution is characterized by $\langle\tau\rangle$, the mean timescale of the process, which could be estimated experimentally.

Using this distribution for Eq. (3.11) we obtain an asymptotic behavior for $t \to +\infty$ for the stationary correlation function of the velocity given by:

$$R(t) = \langle D_V\rangle\langle\tau\rangle\frac{\Gamma(\alpha+1)}{\Gamma(1-\alpha)}\Big(\frac{t}{\tau_*}\Big)^{-\alpha}, \tag{3.13}$$

which is enough to obtain the desired scaling of the position variance $\sigma_x^2(t) \propto t^\phi$, with $\phi = 2 - \alpha$. Note that in the limit in which $\alpha = 1$ we recover the classical correlation function:

$$R(t)_{\alpha=1} = \langle D_V\rangle\tau_* e^{-t/\tau_*}\,. \tag{3.14}$$

3.5 Suitable distributions for D_V

Until the velocity coefficient of diffusion is not random the resulting pdf is still a Gaussian density $G(x, \sigma_x^2(t))$, where the variance $\sigma_x^2(t)$ is the one derived from the correlation function with anomalous time scaling, due to the randomness of the time scale τ. The resulting pdf in the long time limit is:

$$P(x,t;\phi) = \frac{1}{\sqrt{4\pi C t^\phi}}e^{-\frac{x^2}{4Ct^\phi}} \tag{3.15}$$

with $C = \frac{\Gamma(\alpha+1)}{\Gamma(3-\alpha)}\Big(\frac{\Gamma(1/\alpha)}{\alpha}\Big)^{(2-\phi)}\langle\tau\rangle^{(3-\phi)}D_v$.

Including random velocity diffusivity D_V we may derive not Gaussian pdf. From the Lemma 3.1 in [26] we have that the pdf associated to a product of two independent random variables $z = \lambda^\rho z_1$ is:

$$p(z) = \int_0^\infty p_1(z/\lambda^\rho)p_\lambda(\lambda)\frac{d\lambda}{\lambda^\rho}\,. \tag{3.16}$$

Then if we consider $z = xt^{-\phi/2}$, $z_1 = x_\phi t^{-\phi/2}$ and $\lambda^\rho = \sqrt{\Lambda}$ that is equivalent to $x = \sqrt{\Lambda}x_\phi$, with $\Lambda = D_V/D_v$ and we can write:

$$P(\frac{x}{t^{\phi/2}}) = \int_0^\infty P_{x_\phi}\Big(\frac{x}{(t^\phi\Lambda)^{1/2}}\Big)p_2(\Lambda)\frac{d\Lambda}{\Lambda^{1/2}}\,. \tag{3.17}$$

Considering the Gaussian distribution for x_ϕ reported in Eq. (3.15) and the relationship between Λ and D_V, we obtain the following general relation:

$$P(x,t) = \int_0^\infty G_\phi(x, \sigma_x^2(t, D_V))h(D_V)dD_V\,, \tag{3.18}$$

which means that the final probability is the conditional probability respect to the realization of the random variable D_V weighted over the distribution $h(D_V)$.

Assuming different distributions of the velocity diffusivity $h(D_V)$ is it possible to generate different pdfs as the Mainardi or Lévy, which are related to the most known fractional processes in the literature.

In particular, if $p(\Lambda) = M_\beta(\Lambda)$, i.e. the special Wright function known as Mainardi function, we have $h(D_V) = M_\beta(D_V)$ and the resulting pdf is the Mainardi space time distribution with a time stretching:

$$P(x,t) = \frac{1}{2t^{\phi/2}} M_{\beta/2}\Big(\frac{|x|}{t^{\phi/2}}\Big)\,. \tag{3.19}$$

Note that the latter can be seen as the Green function of the time fractional diffusion equation.

Considering $p(\Lambda) = L^{-\alpha/2}_{\alpha/2}(\Lambda)$, i.e. $h(D_V) = L^{-\alpha/2}_{\alpha/2}(D_V)$, extremal Lévy distribution, we obtain that the final pdf is the symmetrical Lévy distribution:

$$P(x,t) = \frac{1}{2t^{\phi/2}} L^0_\alpha\Big(\frac{x}{t^{\phi/2}}\Big)\,. \tag{3.20}$$

This can be seen as the Green function for the space fractional diffusion equation. In this last case we notice that the diffusivity of velocity does not have a finite mean value, which means that the energy necessary to the system to generate such a process should be infinite. This is not realistic in nature but mathematically it is consistent with the fact that the final distribution $P(x,t)$ is a Lévy density and has an infinite position variance.

Introducing a cut-off on $h(D_V)$, the mean value should become finite as well as the position variance in the final distribution and the energy involved in the process. However the analyticity of the solution is lost and the final distribution can only be computed numerically. We expect this numerical solution to be similar, at least in the long time limit, to the distribution related to Lévy Flights (sec. 2.2).

Chapter 4

Numerical Results

First of all in this Chapter it is reported a study of the *pseudo-random number* generators that are considered for the all simulations. A generator of variables distributed according to the α-*Stable* distribution is also described. Different schemes to integrate the classical Langevin equation are studied and used to reproduce the Ornstein-Uhlenbeck process, described in Chapter 1. Finally the simulations suggested from the alternative approach proposed in Chapter 3 are analyzed and discussed, also in comparison with the results from the other methods described in Chapter 2. The numerical simulations are implemented in *Python*.

4.1 Generation of random variables

The generation of random variables is the starting point of this present study. To reproduce a stochastic noise and to be able to extract random variables distributed according to specific distributions is what we need as basic tools to achieve our target. Thus, in this section it is described the development of these tools.

4.1.1 Pseudo random generator

The random numbers generation is something that a computer cannot manage because of its deterministic methods, indeed a real random generator is a tool able to provide a sequence of non deterministic numbers. Thus, we are going to deal with numbers, called *pseudo-random*, that seem random, but they are not and are generated by means of appropriate algorithms. A good sequence of random numbers should be unpredictable and independent so that, the features used to study the goodness of a Pseudo Random Number Generator (PRNG) are respectively *period* and *randomness*. If for the former there is a simple judgment rule, the longer is the period, the better is the sequence, for the latter it is more complicated to confer such a quality to a sequence of

numbers. It is possible to proceed according to the *Von Neumann criterion* which asserts that every random number is equiprobable thus the extraction of N differ numbers has to give rise to a uniform distribution. Together with the two parameters already explained also *efficiency*, *repeatability* and *portability* have to be check in order to verify the PRNG's quality.

In *Python* there are many PRNG already implemented in its library called *random* and the basic one is given by the *Mersenne-Twister algorithm* [17]. The latter was developed by Makoto Matsumoto e Takuji Nishimura in 1997 and it is a particular kind of *Linear congruential generator* (LCG) which became popular thanks to the following characteristics:

- It has a really huge period, $2^{19937} - 1$, which explains the origin of the name: it is a Mersenne prime number like many other constants of the algorithm;
- It allows to generate equiprobable numbers in a 623-dimensional space;
- It is faster than the majority of the LCG;
- It passes many statistic tests.

LCGs use a discontinuous piecewise linear equation defined by the recurrence relation:

$$X_{n+1} = (aX_n + c) \mod m\,. \tag{4.1}$$

There is another LCG that operates in moltiplicative group of integers modulo m, which means that the constant c in (4.1) is equal to zero, called *Lehmer pseudo random number generator* also known as *Park-Miller* algorithm [28]. It has a period highly smaller than the previous, $p = 2^{31} - 1$, but it is really simple to implement.
For our purpose having a such large period is not so important, but it is more important to have a good uniform distribution in order to be sure to have a good randomness of the generated numbers. Thus the two algorithms presented was combined together to obtain a more unpredictable sequence; the former generators is used to extract a number that then becomes the seed of the latter algorithm. The same method is used to generate standard distributed random variables by means of *Box-Muller algorithm* instead of the Park-Miller one. Studies using the $\chi^2 - test$ have been done to check the results of both the two methods.

4.1.2 α-Stable random generator

The generation of α-Stable random variables is critical for our aim, since it allows to obtain the two random parameters we are interested in for the simulations, τ and D_V. As described in Chapter 3, in order to reproduce the physical phenomena we are dealing with these two parameters must obey to specific distribution functions, which

can all be constructed starting from the general case of the α-Stable Distribution. These distributions don't have an explicit analytical form for the pdf thus it is not possible to generate variables extracted from them by means of classical methods like the *inverse transformation method* [1].

Chambers and Mallow [2, 6] have found a direct method to generate extremal Lévy distributed random numbers

$$L^{EXT}_{\alpha,CM} = \frac{\sin[\alpha(r_1+\pi/2)]}{(\cos r_1)^{1/\alpha}}\left\{\frac{\cos[r_1-\alpha(r_1+\pi/2)]}{-\ln r_2}\right\} \quad , \quad 0<\alpha<1\,, \tag{4.2}$$

where r_1 and r_2 are random variables uniformly distributed in $(-\pi/2, \pi/2)$ and $(0, 1)$ respectively. Through lots of draws of this method, it is possible to obtain a histogram of extremal Lévy probability density for assigned parameters values. At small and large argument values the histogram is usually distorted but since we know the analytical asymptotic behavior, the distribution can be fixed replacing the distorted samples by the asymptotic values. One should ensure that this representation, which we will referred to as semi-analytical, is normalized for every value of the parameters. So that are introduced two normalization parameters $k_1(\alpha)$ and $k_2(\alpha)$ in order to have:

$$\int_0^\infty L^{EXT}_\alpha(x)dx = \int_0^{x_n} k_1(\alpha)x'^{-a}e^{-bx'^{-c}}dx' + \sum_{i=n}^{N} L^{EXT}_{\alpha,CM}(x_i)dx_i + \int_{x_N}^\infty \frac{k_2(\alpha)}{x'^{1+\alpha}}dx' = 1\,, \tag{4.3}$$

where $L^{EXT}_\alpha(x)$ is the constructed distribution, the second term on the right-hand is the histogram obtained by the Chambers-Mellow method and the first and last term are the asymptotic form respectively for $x \to 0^+$ and $x \to \infty$, with

$$a = \frac{2-\alpha}{2(1-\alpha)}; \quad b = (1-\alpha)\alpha^{\alpha/(1-\alpha)}; \quad c = \frac{\alpha}{1-\alpha}\,.$$

Note that the normalization constant is needed only for the analytical forms because the numerical one is proved to be already normalized by Chambers[2].

Once the semi-analytical distribution is constructed, it is also possible to obtain a semi-analytical cumulative distribution which can be used to generate the desired random variables by means of the inverse transformation method.

Probability density function of τ

We want that the time scale parameter τ undergoes the distribution in Eq. 3.12 which is reported here for convenience:

$$b(\tau) = \frac{\alpha}{\Gamma(1/\alpha)}\frac{1}{\tau}L^{-\alpha}_\alpha\left(\frac{\tau}{\tau_*}\right), \tag{4.4}$$

[1] It is a basic method for generating sample numbers at random form any probability distribution, given its cumulative distribution function.

where $L_\alpha^{-\alpha}(z)$ is the equal Lévy density with $0 < \alpha < 1$ and $\tau_* = \langle\tau\rangle(\Gamma(1/\alpha)/\alpha)$. In the simulations τ_* is set to one; it physically means that we are selecting a system with a well defined mean of τ, equal to $\langle\tau\rangle = \alpha/\Gamma(1/\alpha)$.

To generate variables according to this distribution we have to take the semi-analytical distribution constructed for the extremal Lévy density and to divide it by the argument itself. We have to introduce an additional normalization constant for each α, thus the distribution is defined as

$$f_\tau(x) = \frac{A(\alpha)}{x} L_\alpha^{EXT}(x)\,. \tag{4.5}$$

Therefore the semi-analytical cumulative function is computed again for this specific case. Now it is possible to generate random variables according to (4.4) just drawing uniform distributed random variables (u), evaluating the semi-analytical cumulative function for these values $(F_\tau(u))$ and then inverting it $(\tau = F_\tau^{-1}(u))$. Note that also the inversion process is done numerically.

Probability density function of D_V

Due to what we saw in Chapter 3, once that an anomalous Gaussian process x_H is generated (in our case through a Langevin approach with random time scales) it is possible to obtain a non Gaussian process x just introducing the randomization of D_V. The pdf of velocity diffusion coefficient $h(D_V)$ does not depend on time and the stochastic variable D_V is independent of τ. Thus, our choses for $h(D_V)$ are linked only to which kind of final stochastic process we want to have:

$$x = \sqrt{\Lambda} x_H \quad \text{with} \quad 2H = \Phi\,. \tag{4.6}$$

Processes fractional in space can be reproduced considering the following diffusion equation fractional in space:

$$\frac{\partial P(x,t)}{\partial t} = \nu H t^{\nu H - 1} \frac{\partial^\nu P(x,t)}{\partial |x|^\nu} \quad 0 < \nu < 2\,. \tag{4.7}$$

Its solution is a Lévy function and as we saw in Chapter 3, in order to obtain processes according to Eq. (4.7) we can define D_V as:

$$h(D_V) = L_{\nu/2}^{EXT}(D_V)\,. \tag{4.8}$$

From this processes we can obtain as a special case the *Space time fractional diffusion.*

Processes fractional in time can be instead described by the *Erdèly-Kober time Fractional Diffusion equation*

$$\frac{\partial P(x,t)}{\partial t} = \frac{2H}{\beta} t^{2H-1} D_{2H/\beta}^{(\beta-1),(1-\beta)} \frac{\partial^2 P(x,t)}{\partial x^2}\,. \tag{4.9}$$

Eq. (4.9) has a Mainardi function as solution. In this case the velocity diffusion coefficient has to be defined in the following way:

$$h(D_V) = M_\beta(D_V)\,. \tag{4.10}$$

Random variables according to the distributions reported in (4.9) and (4.10) can easily be constructed thanks to the generator described above in this section. In the space fractional case we directly have an extremal Lévy function while for the time fractional case we can use the same generator remembering that:

$$M_\beta(x) = \left[L_\beta^{EXT}(x)\right]^{-\beta}. \tag{4.11}$$

4.2 Time discrete approximations of stochastic processes

Stochastic simulations typically require the calculation of many different realizations of the approximating process, so efficiency and stability are crucial factors to be taken in account. Furthermore we have to construct an algorithm to solve the Langevin equation suitable for all the different cases we are interested in.

A stochastic process x satisfying the scalar stochastic differential equation:

$$dx = a(x,t)dt + b(x,t)dW \tag{4.12}$$

is considered, with the initial value $x_{t_0} = x_0$ and $t_0 \leq t \leq T$. Given a discretization of the time interval $[t_0, T]$, for every discretization time $t_n = t_0 + n\Delta t$ we are interested in the approximated solution y_n of the process described by (4.12). Different schemes can be defined for this aim and to choose the best one for our studies is what we will do all along this section.

A criterion to judge a stochastic approximation's quality (which in the numerical field is described by the concept of *accuracy*) can be established depending on what one is interested in. Namely, it is possible to distinguish two different tasks:

- to obtain a good *pathwise approximation*;
- to obtain a good approximation for the expectation values.

To these aims two important concepts are respectively connected, the *Strong Convergence* and the *Weak convergence*. We shall say that a general time discrete approximation y^δ, where δ is the maximum step size, *converges strongly* to x at time T if:

$$\lim_{\delta\to 0} E\big(|x_T - x^\delta(T)|\big) = 0\,. \tag{4.13}$$

In order to asses and compare different time discrete approximations a rate of strong convergence $\gamma > 0$ is defined. We shall say that a time discrete approximation y^δ *converges strongly with order* $\gamma > 0$ at time T if there exists a positive constant C, which do not depend on δ, and a $\delta_0 > 0$ such that:

$$\epsilon(\delta) = E\big(|x_T - y^\delta(T)|\big) \leq C\delta^\gamma \quad , \quad \forall \delta \in (0, \delta_0)\,. \tag{4.14}$$

As we con see from Eq. (4.13) and (4.14) the strong convergence criterion is based on an error evaluation directly connected to the pathwise approximation, given by:

$$\epsilon = E\big(|x_T - y(T)|\big)\,.$$

Is it also possible to define the approximation error with respect to the mean:

$$\epsilon_\mu = E\big(y(T)\big) - E\big(x_T\big)\,.$$

In this case we shall say that a general time discrete approximation y^δ *converges weakly* to x at time T with respect to a class $\mathcal{C}$ of test functions if we have

$$\lim_{\delta \to 0} \big|E\big(g(x_T)\big) - E\big(g(y^\delta(T))\big)\big| = 0 \quad , \quad \forall g \in \mathcal{C}\,, \tag{4.15}$$

and the order of *weak convergence* is $\eta > 0$ if

$$\big|E\big(g(x_T)\big) - E\big(g(y^\delta(T))\big)\big| \leq C\delta^\eta\,. \tag{4.16}$$

The approximation convergence alone cannot guarantee good results for a scheme due to problems caused by the error propagation. We need also a counterpart to the deterministic concept of numerical stability for the stochastic approximation. We shall say that a time discrete approximation y^δ is *stochastically numerically stable* for a given stochastic differential equation if for any finite interval $[t_0, T]$ there exists a positive constant Δ_0 such that for each $\epsilon > 0$ and each $\delta \in (0, \Delta_0)$

$$\lim_{|y_0^\delta - \bar{y}_0^\delta| \to 0} \Big\{ \sup_{t_0 \leq t \leq T} P\big(|y_t^\delta - \bar{y}_t^\delta| \geq \epsilon\big) \Big\} = 0\,, \tag{4.17}$$

where $\bar{y}^\delta$ represents another discrete approximation characterized by the value $\bar{y}_0^\delta$ at the initial time t_0.

4.2.1 Taylor approximations: Euler-Maruyama and Milstein schemes

In the integration schemes reported here it is used the stochastic Taylor expansion [8] where the truncation is determined by the order of convergence. Both the weak and

strong orders convergence determine the truncation that must be used but the one for the weak convergence in general involves less terms. The *Euler* scheme, also known as *Euler-Maruyama* scheme, represents the simplest one and it generally attains the order of strong convergence $\gamma = 0.5$ and the order of weak convergence $\eta = 1$. In the 1-dimensional case this scheme has the form

$$y_{n+1} = y_n + a\Delta t + b\Delta W\,, \tag{4.18}$$

where Δt is the length of the time discretization subintervals and ΔW is the increment of the Wiener process.

The *Milstein* scheme has a strong convergence of order 1 and in this sense can be regard as the proper generalization of the deterministic Euler scheme. It can be written as:

$$y_{n+1} = y_n + a\Delta t + b\Delta W + \frac{1}{2}bb'\big((\Delta W)^2 - \Delta t\big)\,. \tag{4.19}$$

In our studies we will always have an additive noise independent from t so, in fact, these two schemes, Eq. (4.18) and Eq. (4.19), turn out to coincide for our purpose and they give:

$$\begin{cases} x_{n+1} = x_n + v\Delta t \\ v_{n+1} = (1 - \dfrac{\Delta t}{\tau})v_n + \sqrt{2D}\Delta W\,. \end{cases} \tag{4.20}$$

4.2.2 Derivative free schemes

Following the Taylor approximation if we want to increase the convergence order, we should introduce higher order derivatives of the stochastic equation coefficients. Here we examine schemes which avoid the use of derivatives in much the same way that *Runge-Kutta* schemes do in the deterministic case. The idea is simply to replace the derivatives of the Taylor approximation by the corresponding difference ratios; these differences require the use of supporting values of the coefficients at additional points. For example we can consider the following autonomous scheme due to *Platen* [8] with order of strong convergence 1.5 and it is reported here only for the case of additive noise:

$$y_{n+1} = y_n + b\Delta W + \frac{1}{2\sqrt{\Delta t}}\{a(\bar{y}_+) - a(\bar{y}_-)\}\Delta Z + \frac{1}{4}\{a(\bar{y}_+) + 2a + a(\bar{y}_-)\}\,, \tag{4.21}$$

with

$$\bar{y}_\pm = y_n + a\Delta t \pm b\sqrt{\Delta t}\,, \tag{4.22}$$

and the additional random variable ΔZ represents the double integral of the Wiener process which is normally distributed with zero mean and variance $E((\Delta Z)^2) = (\Delta t)^3/3$.

The latter can be generate from two independent normally distributed variables, u_1 and u_2, by means of the transformation:

$$\Delta Z = \frac{1}{2}(\Delta t)^{3/2}\Big(u_1 + \frac{1}{\sqrt{3}}u_2\Big)\,. \tag{4.23}$$

In the same way it is also possible to construct an implicit derivative free scheme. It is consider for example an autonomous scheme with order of strong convergence 1.5, like the explicit one just discussed.

$$y_{n+1} = y_n + b\Delta W + \frac{1}{2}\{a(y_{n+1}) + a\} + \frac{1}{2\sqrt{\Delta t}}\{a(\bar{y}_+) - a(\bar{y}_-)\}\big(\Delta Z - \frac{1}{2}\Delta W \Delta t\big)\,, \tag{4.24}$$

where ΔZ is always a random variable obtained by (4.23) and the supporting values are

$$\bar{y}_\pm = y_n + a\Delta t \pm b\sqrt{\Delta t}\,. \tag{4.25}$$

Implicit schemes usually have a wide range of step sizes suitable for the approximation of dynamical behavior, in particular with many different time scales, without the excessive accumulation of unavoidable initial and roundoff errors. On the other hand, in implementing an implicit scheme we need to solve an additional algebraic equation at each time step and, even if there is no accumulation of errors, it can become imprecise providing results far from the real process.

4.2.3 Multi-step scheme

Multi-step method are often more efficient computationally than one-step method of the same order because they require only one new evaluation of the right hand side of the differential equation for each iteration thus to take in account at least one of these is worthwhile.

Considering our system in the phase space, a 2-step scheme suitable for the x variable can be obtained starting from the *Milstein* scheme

$$\begin{cases} x_{n+1} = x_n + v_n\Delta t \\ v_{n+1} = v_n + a(t_n)\Delta t + b\Delta W\,. \end{cases} \tag{4.26}$$

Solving the first equation we have $v_n = (x_{n+1} - x_n)/\Delta t$ and insert it into the second we obtain a 2-step scheme for x given by:

$$x_{n+2} = \Big[2 - a(t_n)\Delta t)x_{n+1}\Big] - \Big[1 - a(t_n)\Delta t\Big]x_n + b\Delta W\,. \tag{4.27}$$

This scheme is thus equivalent to the 2-dimensional *Milstein* scheme reported in (4.26) and we can use its first equation both as a starting routine and to calculate approximation of the second variable.

4.2.4 Δt-variable method

Following from the Thomson's work [33] it is also presented a method with a variable temporal step. To choose a new temporal step at each time allows us to take into account the phase space state in which the system is and to decide the next step in order to avoid the particle to make a large change of its position. In this way we ensure to reproduce the sample paths with a physical perspective which is going to be essential for the reproduction of anomalous dynamic, as we will see. Starting from Eq. (4.12) the temporal step is selected to be:

$$\Delta t = \min\left\{\frac{0.05}{b}, \frac{0.1}{|a|}\right\}. \tag{4.28}$$

The latter is a dimensionless relation of which the dimensional version can be written as

$$\Delta t = \min\left\{\frac{0.05\sigma_v^2}{b}, \frac{0.1\sigma_v}{|a|}\right\}. \tag{4.29}$$

The problem using this method is that every realization has its own discretization of the temporal interval so, if we want to compare each other the sample path we need to define some observation times. The idea is thus to let the simulation of each trajectory proceed until it reaches or just exceeds one of the observation times, then in the first case we simply save the value obtained while, in the second case, we make an interpolation of the values obtained in the instants previous and after the observation time and we store this new value. The observation times are chosen to be 10 in every decade established by the value of τ, from $10^{-1}\tau$ to $10^3\tau$.

Every scheme previous described can be adapted to this Δt-variable method; different proves have been done but here, for convenience, it is reported only the implementation of this method within the explicit Runge-Kutta scheme which provides good results in term of accuracy and computational efficiency.

4.3 Normal diffusion simulations

The first step of the numerical simulations is to reproduce the standard diffusion model, with all its features in order to test all the schemes implemented.

4.3.1 Wiener process

We have already introduced the standard Wiener process in Chapter 1 for the mathematical description of Brownian motion. Recalling it we define a standard Wiener process $W(t)$ to be a Gaussian process with independent increments such that

$$W(0) = 0 \quad \langle W(t)\rangle = 0 \quad \langle (W(t) - W(t'))^2\rangle = t - t', \quad \forall\, t' \leq t\,. \tag{4.30}$$

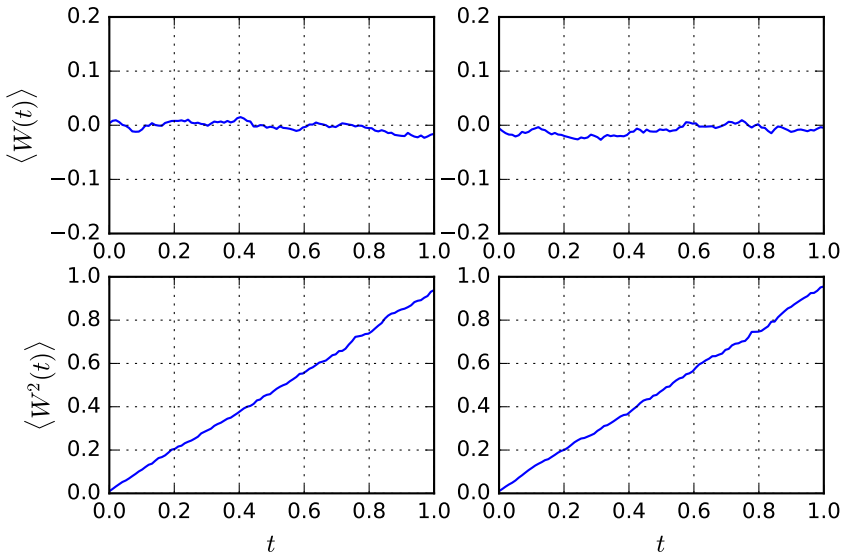


Figure 4.1: Wiener process: mean and variance. On the left the process obtained starting from uniform distributed variables, on the right the one from normally distributed variables.

It is possible to approximate a standard Wiener process by a scaled random walk taking independent, equally probable steps of length $\pm\sqrt{\Delta t}$ at the end of each subinterval of the time interval. Starting from uniform distributed variables x_i, then we define

$$S_N(t_n) = (x_1 + x_2 + \cdots + x_N) \implies W_N(t_n) = S_N(t_n)\sqrt{\Delta t}\,. \tag{4.31}$$

By the Central Limit Theorem $W_N(t)$ converges in distribution as $N \to \infty$ to a process with independent increments satisfying (4.30), that is a standard Winer process. To ensure that the Wiener process has zero mean and variance equal to 1 the uniform distributed variables are defined in the time interval $[-\frac{1}{2}, \frac{1}{2}]$ and rescale by a factor $\sqrt{12}$:

$$K \int_{-1/2}^{1/2} x^2 p(x) dx = K \int_{-1/2}^{1/2} x^2 dx = K \frac{1}{12} = 1 \implies K = 12\,.$$

It is alo reported another process obtained directly by summing standard distributed variables instead of uniform distributed variables; this process is thus Gaussian by definition in every moments and not only in the long limit. The results for both cases are reported in Figure 4.1 and 4.2.

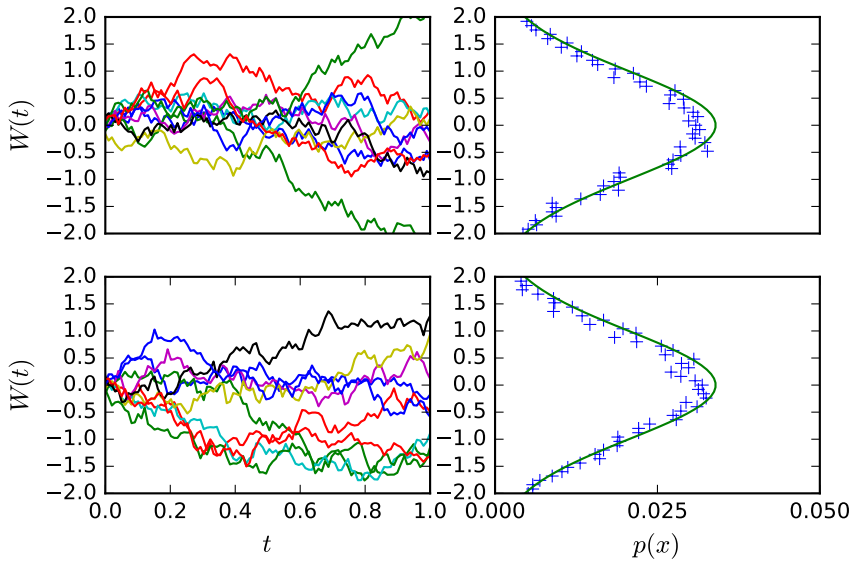


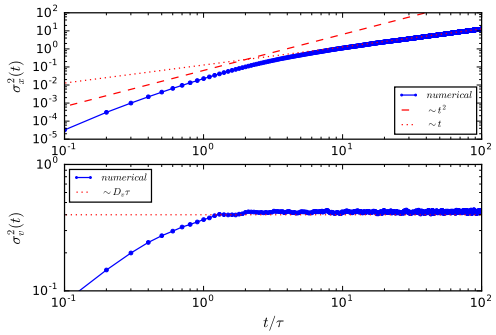
Figure 4.2: Wiener process: sample paths and pdf. On the top the process obtained starting from uniform distributed variables, on the bottom the one from normally distributed variables.

4.3.2 Ornstein-Uhlenbeck process

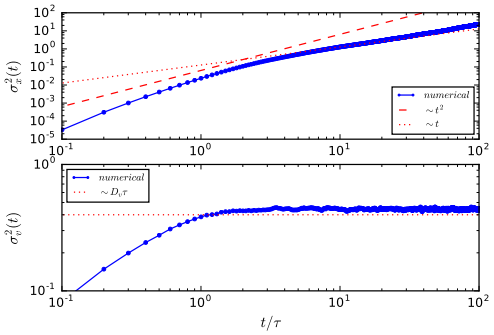
The integration schemes described in the previous section are used to simulate the Ornstein-Uhlenbeck (OU) process described in Chapter 1. Every simulation has 10000 realizations with a temporal step equal to $4 \cdot 10^{-3}$, the velocity diffusion coefficient D_v is set to 1, the initial time and position are set to 0 and $\tau = 0.4$. The only exception is for the Δt-variable method which has been implemented with $\tau = 0.04$ and a longer temporal interval. As far as the initial velocity is concerned different conditions have been studied.

We start from the case with the initial velocity equal to zero; the displacement and velocity variance obtained through different integration schemes is reported in Figure 4.3.

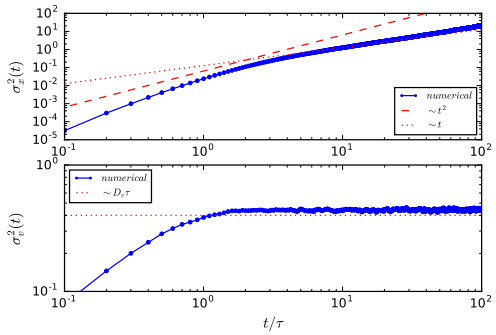
The latter shows that all the different schemes reproduce correctly the main characteristics of the stochastic process.The red lines in the plots represent the analytical behaviors found in Chapter 1. The long-time trends for the both variances are satisfied while the trend for small time values in the displacement variance is not fulfilled. This is not a numerical error, but is only due to the initial condition chosen for the velocity. As a metter of fact setting this value to zero means that we start looking and studying the system before it reaches its stationary state where the analytical trends found are effective. Going on with time, the system manages to reach the equilibrium state after some



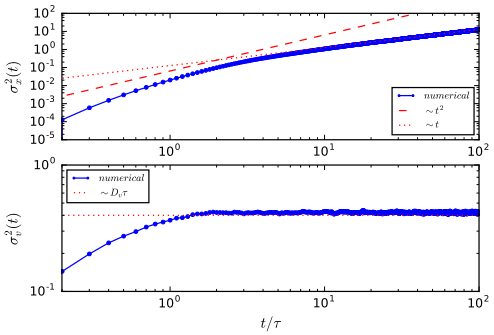
(a) *Milstein method.*



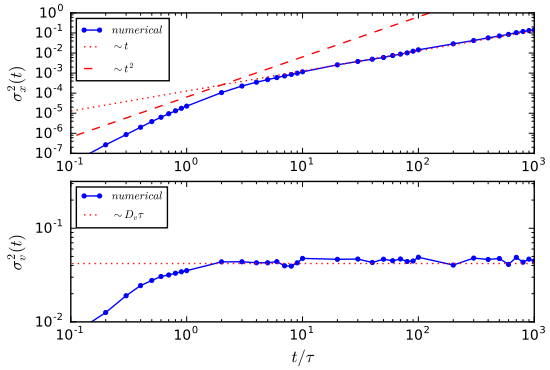
(b) *Explicit Runge-Kutta method.*



(c) *Implicit Runge-Kutta method.*



(d) *2-step method.*



(e) Δt*-variable method.*

Figure 4.3: Position and velocity variance of the Langevin equation trajectories with $D_v = 1$, $\tau = 0.4$ and $v_0 = 0$.

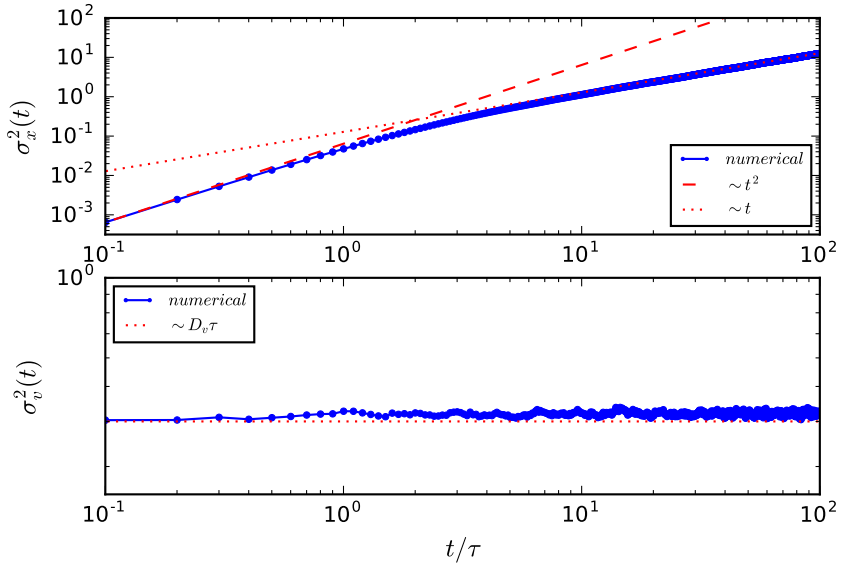
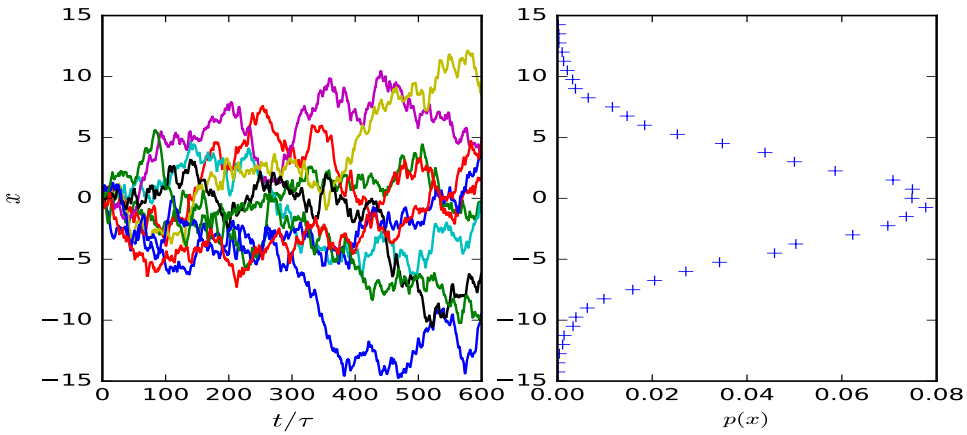


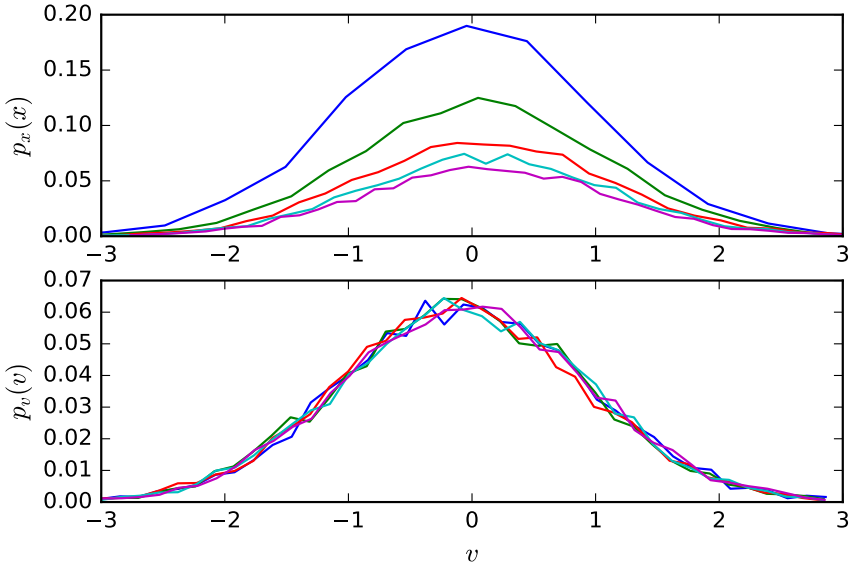
Figure 4.4: Position and velocity variance of the Langevin equation trajectories with $D_v = 1$, $\tau = 0.4$ and $v_0 \sim N(0, \sigma_{v,eq})$.

unities of τ where we can observe the long-time trends only because of the logarithmic scale.

In order to verify also the trend for short time we can take advantage of the knowledge of the velocity equilibrium distribution, which is the Maxwell-Boltzmann distribution. Thus, another simulation of the OU process is reported with the same parameter, except for the initial velocity which has been taken from a Gaussian distribution with zero mean and variance equal to $\sigma_{v,eq}^2 = D_v\tau$. Only the results with one integration scheme, the 2-step method, are presented in Figure 4.4. In Figure 4.4 it is possible to observe both the two trends thanks to the change of the initial conditions; our system is now at the thermodynamical equilibrium since the first moments, so we are able to evidence the complete dynamic in its stationary state. Figure 4.5 showes some sample paths together with the probability distribution function which is a Gaussian as expected. In particular it is possible to notice how in Figure 4.5-(b), as we can see also in Figure 4.3, the velocity *pdf* keeps the same variance for all the times while the displacement *pdf* variance grows, going through a sort of scattering. To conclude Figure 4.6 shows the plot of the velocity correlation function for this case, in which we expect to have the stationary part only. The numerical data perfectly fit the analytical trend defined by Eq. (1.13)



(a) *Sample paths and pdf.*



(b) *Displacement and velocity pdf at different time values.*

Figure 4.5: Trajectories and pdf of the Langevin equation with $D_v = 1$, $\tau = 0.4$ and $v_0 \sim N(0, \sigma_{v,eq})$.

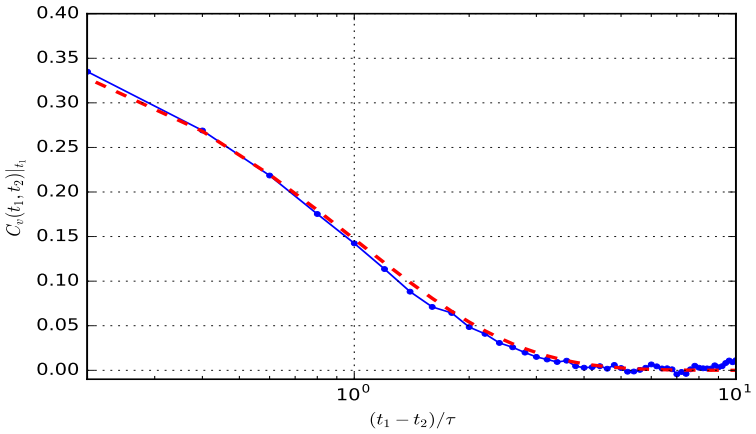


Figure 4.6: Velocity correlation function of the Langevin equation trajectories with $D_v = 1$, $\tau = 0.4$ and $v_0 \sim N(0, \sigma_{v,eq})$.

4.4 Fractional Diffusion Simulations

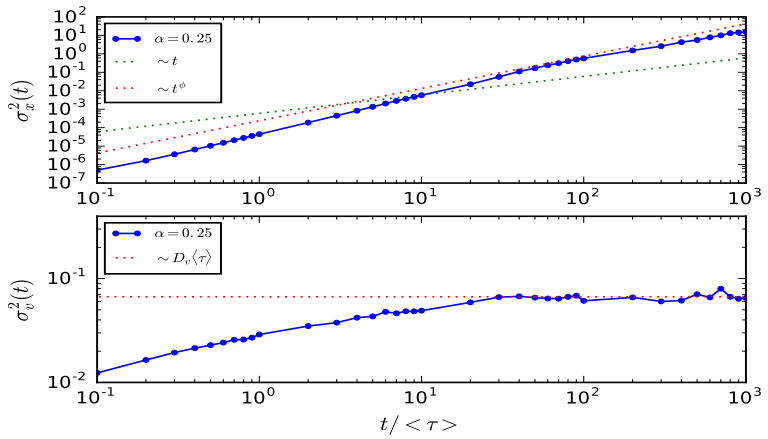
The fractional dynamics involves lots of cases, as we saw in Chapter 2, so that the numerical simulations have to be split. The first division is of course between *subdiffusion* and *superdiffusion*. In Chapter 3 we found out that to reproduce the former we need to add an oscillating potential to the *Langevin equation*, which we chose for simplicity to be harmonic. Due to the need of this modification, to verify and test the model presented in Chapter 3 it is decided to start from the *superdiffusion* case which allows us to avoid changes to the equation structure and it just requires the introduction of the random parameters. Therefore in this section are reported studies on *superdiffusion* only. The *subdiffusive* case is let as future research motivated by the promising results achieved in the present thesis.

4.4.1 Distribution of τ and anomalous time scaling

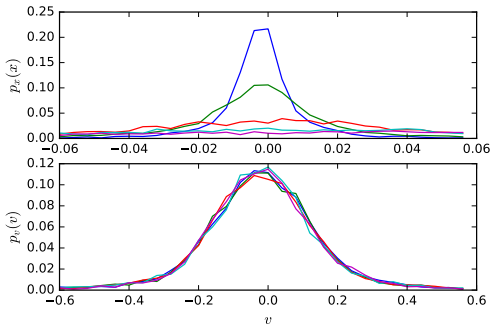
Since the two parameters D_V and τ are considered independent, we can start from the randomization of the time scale leaving the diffusivity velocity coefficient as a fixed value. In this particular case the process we expect to obtain is still Gaussian, because there are no changes of the noise, but with an anomalous time scaling for the position variance:

$$\sigma_x^2(t) \sim t^{\phi}, \quad 1 < \phi < 2\,. \tag{4.32}$$

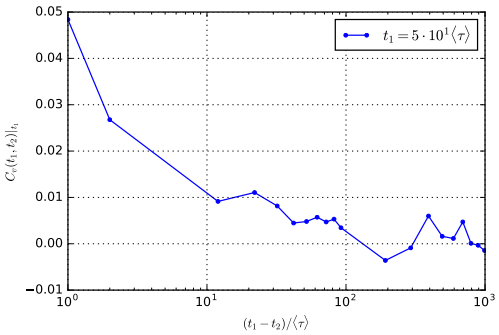
The scale parameter ϕ depends on the distribution from which we take the values of τ, which are obtained as described in the first section of this Chapter. The distribution of τ depends on a parameter α which, as we saw, is linked to ϕ by the relation $\phi = 2 - \alpha$.



(a) *Displacement and velocity variance.*

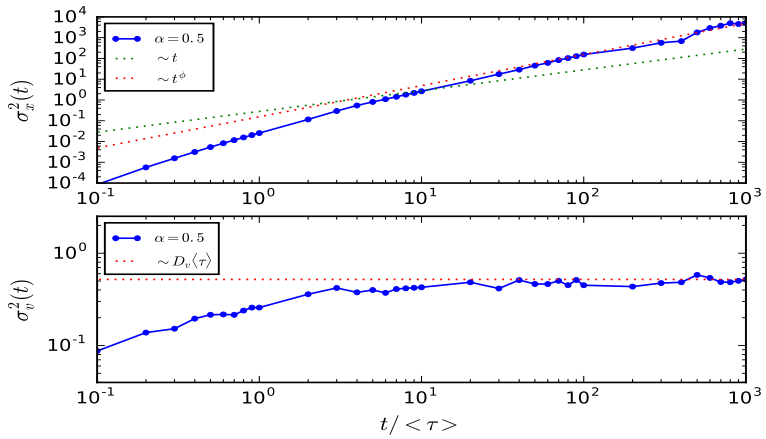


(b) *Displacement and velocity pdf at different times.*

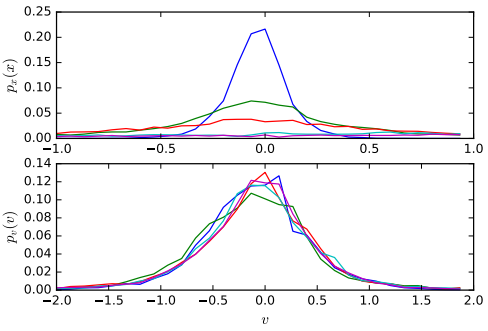


(c) *Velocity correlation function.*

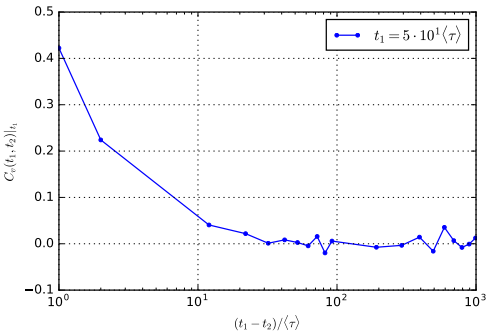
Figure 4.7: $D_v = 1$, $\alpha = 0.25$ and $v_0 = 0$.



(a) *Displacement and velocity variance.*

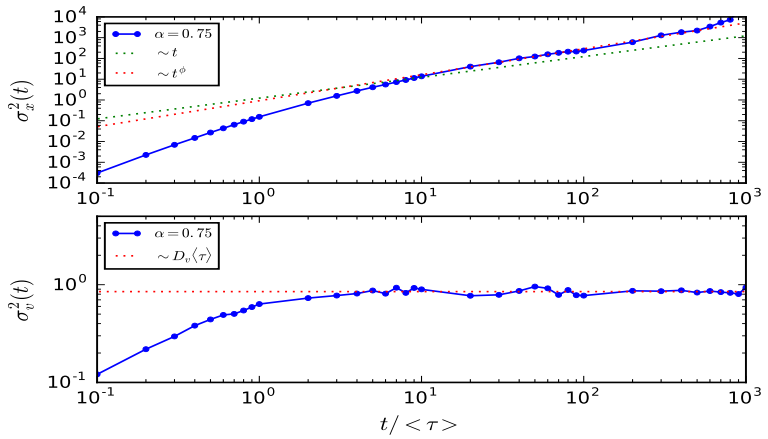


(b) *Displacement and velocity pdf at different times.*

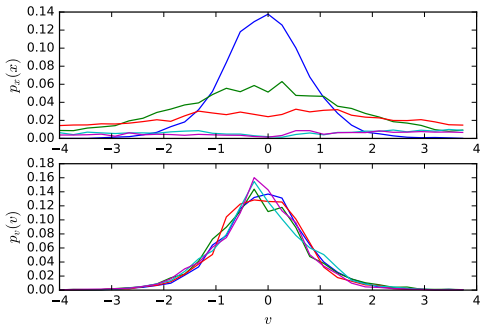


(c) *Velocity correlation function.*

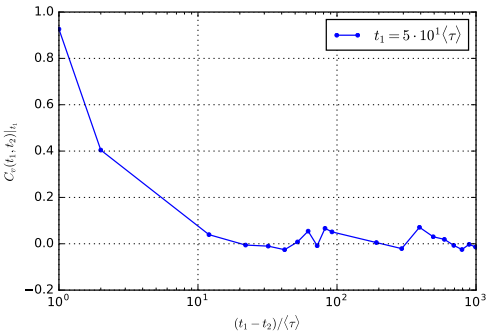
Figure 4.8: $D_v = 1$, $\alpha = 0.5$ and $v_0 = 0$.



(a) *Displacement and velocity variance.*



(b) *Displacement and velocity pdf at different times.*



(c) *Velocity correlation function.*

Figure 4.9: $D_v = 1$, $\alpha = 0.75$ and $v_0 = 0$.

The integration scheme largely conveys the variability of τ and so, in order to optimize the computational time ,only the Δt-variable method is used. In its evaluation of the temporal step this method takes in account the value of τ. Furthermore we faced problems of stability for extremely small value of τ so a rather drastic solution for this purpose is selected: to put a cutoff value in the extraction of τ. This condition influences the building of a good sample of τ that has to be extracted from the suitable distribution and then used for the simulation. On the other hand we might say that this could not affect the success of the simulations since the trends in which we are interested depend only on the average of the temporal scales set. Thus, choosing a sample with a little bit different mean should only lead to different stationary values related to the effective average. The simulations obtained with the Δt-variable method are reported and discussed for different values of α: 0.25, 0.5, 0.75.

Figures 4.7, 4.8 and 4.9 show the main features of the generated processes. In boxes (a) it is possible to observe the trends of position and velocity variance. Both reach their stationary trends in the same moment, as we expect, and in particular we pay attention to the moment in which the system reached its stationary state. Comparing it with the one of the OU process it is possible to notice that in general it is higher and that while α increases, it decreases. This behavior agrees with the fact that while α is growing we approach to the standard diffusion because the pdf of τ approach to a *Dirac delta*. Thus, the presence of random media causes a delay in reaching the stationarity that can be easily explained thinking that the stationary state corresponds to that state in which each realization is relaxed. So we need to wait until all values of tau are over.

In boxes (c) it is possible to observe the velocity correlation functions for a fixed moment t_1, which is selected ensuring that in this moment the system has already reached the stationary state, and t_2 variable in $[t_1, T]$. Figure 4.10 show the velocity correlation function for all the three cases studied. Note that for each value of α the trend drawn

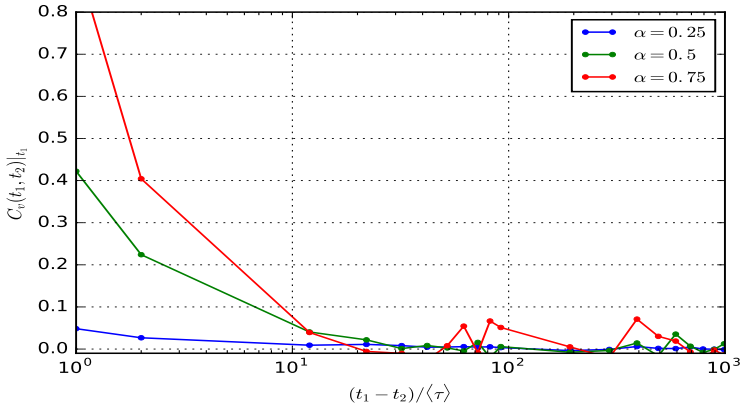
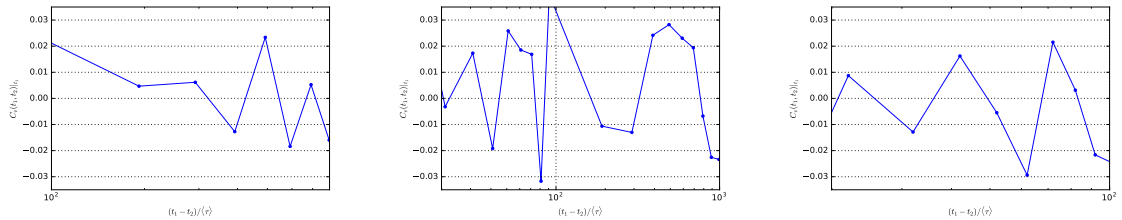


Figure 4.10: Velocity correlation function for different values of α.

by the numerical data is decreasing and monotonous, as expected. It is interesting to observe how the scale of the values changes from one case to the other. In particular, recalling Eq. (3.13), we can link the maximum value of the velocity correlation function to the product $D_v\langle\tau\rangle$ which is deeply related to the energy of the analyzed system, as well as for the standard diffusion case. This observation highlight how in the approach we are studying the parameters probability distribution really characterized the medium in which the diffusion occurs.



(a) $\alpha = 0.25$. (b) $\alpha = 0.5$. (c) $\alpha = 0.75$.

Figure 4.11: Numerical error evaluation from the oscillation of the correlation function tail

.

Furthermore we can consider the oscillations of the difference between the tails of these correlation functions and the analytic behaviours evaluated through Eq. (3.13), to estimate the numerical error of the used scheme. They are shown in Figure 4.11 which allows to evaluate the numerical error around 10^{-2}.
As far as the Gaussianity is concerned a more in-depth study is reported below.

4.4.2 Guassianity study

A critical point of our study is to clarify that with the randomization of the parameter τ we only introduce an anomalous time scaling, showed in Figure 4.7, 4.8 and 4.9, without losing the Gaussianity of the process for every temporal moments. We take into consideration the *Central Limit Theorem*, which is reported below:

Theorem 2 (Central Limit Theorem)**.** *Let $x_1, x_2, \ldots, x_N$ be a set of N independent random variables and each x_i have an arbitrary probability distribution $P(x_1, ..., x_N)$ with mean μ_i and a finite variance σ_i^2. Then the normal form*

$$S_N = \frac{\sum_{i=1}^{N} x_i - \sum_{i=1}^{N} \mu_i}{\sqrt{\sum_{i=1}^{n} \sigma_1}}$$

has a limiting cumulative distribution function which approaches a normal distribution. If conversion to normal form is not performed, then the variable

$$x = \frac{1}{N}\sum_{i=1}^{N} x_i$$

is normally distributed with mean $\mu_x = \langle \mu_i \rangle$ *and variance* $\sigma_x^2 = \langle x_i^2 \rangle - \langle x_i \rangle^2$.

Our system is made by a set of 10000 realizations, each one with a specific value of τ which remains constant for all the simulation time. This means that every simple path is essentially an OU process with its specific temporal scale, different from the one of all the other realizations. Thus, it suggests that every trajectory in the phase space is, at every moment, a Gaussian process with its own mean and variance.

If we now take into account the distribution of the entire system for a fixed time we essentially have an ensamble of normally distributed random variables, each one taken from its own Gaussian distribution, exactly what it is described by the Central Limit Theorem. So the latter ensures that the process obtained is Gaussian in every moment.

To prove it numerically we can provide both a fit of our data with a Gaussian and results from statistical tests. The most used test to prove that a sample of data is extract from a specific distribution is the χ^2-test. This test compares the observed frequencies with the expected ones through the computation of

$$\chi^2 = \frac{1}{N}\sum_{i=1}^{N} \frac{(f_{obs} - f_{exp})^2}{f_{exp}} \,,$$

which undergoes a χ^2-distribution. Statistical tables are then provided to translate the χ^2-value obtained in a level of rejection or acceptance of the null hypothesis H_0 (the sample is extracted from a Gaussian distribution).

Note that this test requires the knowledge of the theoretical distribution of each variables in order to compute the expected frequencies. In our case these distributions vary at each time and we cannot manage to estimate them unless we focused the attention on the stationary state of the system. In this case we have an evaluation of mean and variance. It is worthwhile to observe that even in the stationary case we cannot be sure that every trajectory is thermalized, in particular for those with high value of τ.

Due to this we follow a different approach for the application of the χ^2-test. Instead of converting each variables to the normal form using the evaluation of mean and variance, we just take all the variables as they are and then we convert the obtained distribution to a normal one by means of mean and variane values compute directly from the sample in exam. In this way we manage to compare the final distribution with a normal one, with zero mean and variance 1.

Actually the system we are analyzing is really more complicated than the one we described above. Each variable involved in the distribution computation is itself a sum

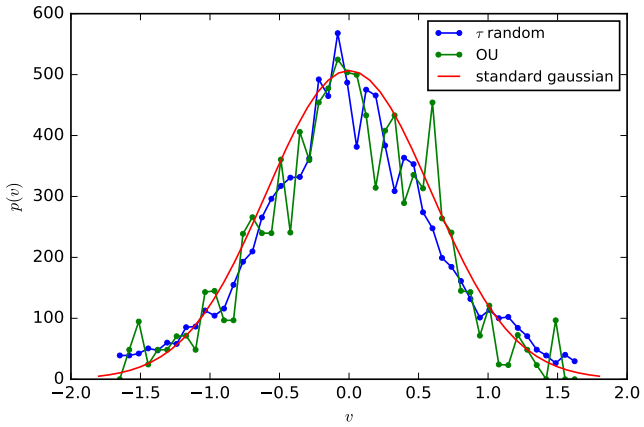


Figure 4.12: Velocity pdf of the Langevin equation trajectories in comparison with the pdf of the process obtained with τ random. In both cases $D_v = 1$ and $v_0 = 0$.

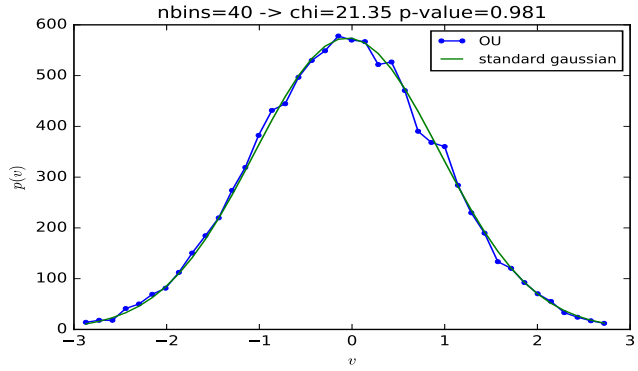
t	W_{OU}	W_τ
$10 \cdot \langle\tau\rangle$	0.90	0.89
$100 \cdot \langle\tau\rangle$	0.91	0.89
$500 \cdot \langle\tau\rangle$	0.90	0.89

Table 4.1: Shapiro-Wilk test results.

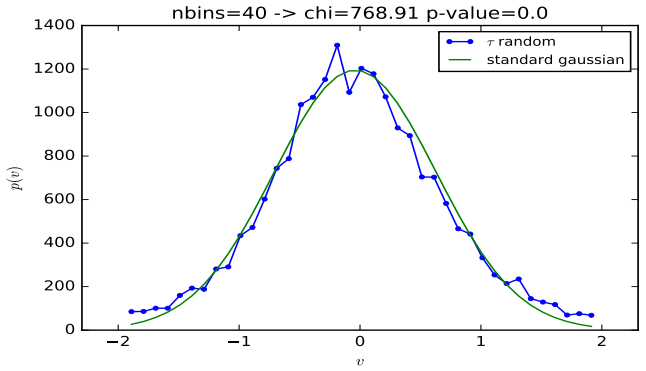
of many (we neither know how many) other random variables defined in relation with each time temporal step. Thus, taking a fixed observation time, we have 10000 variables, which we know that in theory they are gaussian, that are obtained as sum of other random variables with different distributions. Due to this even for the OU process the distributions obtained are very noisy and the χ^2-test cannot provide good results. Anyway in Figure 4.12 it is possible to see that both the OU process and the process with random τ approach the normal distribution just in the same way.

To ensure that this noisy results is really due to the integration scheme with Δt-variable method it is showed in Figure 4.13 the same results obtained with the simple 2step method, for the OU process and the τ random process respectively.

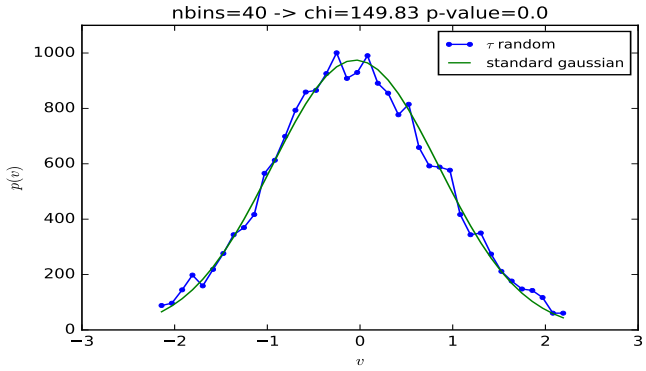
Since in these cases the χ^2-test loses significance for the reasons previous reported, also a non parametric test, the *Shapiro-Wilk test*, has been computed. By means of this we avoid the need of a knowledge about the theoretical distribution and we just verify if our sample is extracted from a normal distribution. The results of this test is reported in Table 4.1; the closer is the test result to 1, the higher is the probability that our sample belongs to a normal distribution .



(a) *Velocity pdf of the Langevin equation trajectories with* $\tau = 0.04$ *,* $D_v = 1$ *and* $v_0 = 0$.



(b) τ *random process pdf with* $\alpha = 0.5$*,* $D_v = 1$ *and* $v_0 = 0$



(c) τ *random process pdf with* $\alpha = 0.75$*,* $D_v = 1$ *and* $v_0 = 0$

Figure 4.13

4.4.3 Distributions of D_V: fractional processes

Through the randomization of τ we menage to reproduce anomalous diffusion processes characterized by position and velocity variance scaling with power laws and Gaussian pdf. Now we introduce the randomization of D_V in order to obtain processes with the same anomalous scalings but with non Gaussian pdf. In this Section we deal with two different cases, *Erdèly-Kober* fractional diffusion and processes fractional in space. These two cases can also be combined together to obtain the more general case of fractional diffusion in space-time. A first example of the changes reported by the position pdf through the randomization of D_V is showed in Figure 4.14. We can see this plots as an indirect proof of the Gaussianity of the samples obtained with the randomization of τ. As a matter of fact the first pdf in Figure 4.14 display itself to be transparent, giving rise to final pdfs totally defined by the distribution chosen for the D_V. If the pdfs obtained through the simulations described in the section above were not be Gaussian, this would not happen.

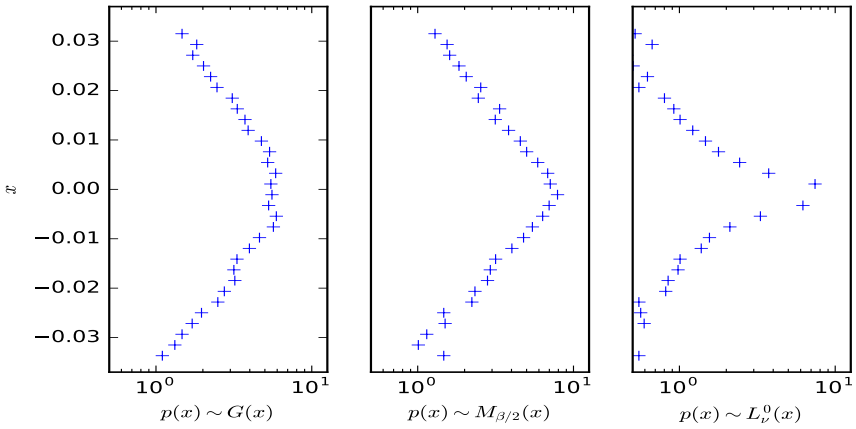


Figure 4.14: Pdfs of x for $\alpha = 0.5$ and three different cases of D_V.

Erdèly-Kober fractional diffusion

To obtain *Erdèly-Kober* fractional diffusion the velocity diffusion coefficient is chosen according to a Mainardi function with the typical parameter, which we referred to as β, that varies from 0 to 1. 10000 different random variables are generated to be combined with the trajectories obtained before, as defined in Eq. (4.6). In this way it is generated a stochastic process with a distribution given by:

$$P(x;t) = \frac{1}{2t^{\Phi/2}} M_{\beta/2}\left(\frac{|x|}{t^{\Phi/2}}\right). \tag{4.33}$$

The asymptotic behavior of the new realizations pdf is studied in comparison with the analytical asymptotic expansion of Eq. (4.33), which is reported below:

$$M_{\beta/2}(|x| \to +\infty) \sim |x|^a e^{-b|x|^c}\,, \tag{4.34}$$

with $a = (\beta - 1)/(2 - \beta)$, $b = (2 - \beta)2^{-2/(2-\beta)}\beta^{\beta/(2-\beta)}$ and $c = 2/(2 - \beta)$. Figure 4.15 shows the results of these comparisons for different values of β and α.

The pdf is symmetric so that it is proposed in some cases the left tail and in other the right one in order to show both. As we can see from Eq. (4.34) the tails present an exponential trend weighted by a power of x. This trend leads to a so fast decay, especially for small values of α, that our data immediately reach values in which we cannot manage to see in a precise way the asymptotic behavior due to the numerical error. Anyway it is possible to notice that when α increases we are able to stretch to spatial interval and the behavior can be better observed.

Space fractional diffusion

Space fractional diffusion processes are generated by means of D_V distributed according to an extremal *Lèvy* function $L^{EXT}_{\nu/2}$, in order to obtain:

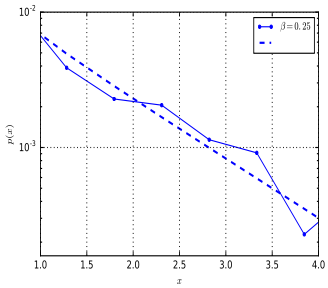
$$P(x;t) = \frac{1}{2t^{\Phi/2}} L^0_\nu\Big(\frac{|x|}{t^{\Phi/2}}\Big) \quad . \tag{4.35}$$

The asymptotic expansion of the *Lèvy* function is given by:

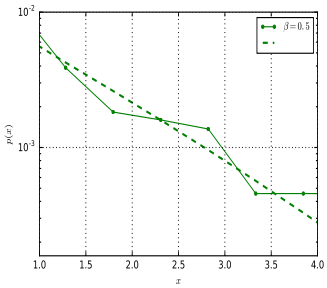
$$L^\theta_\nu(|x| \to +\infty) \sim \frac{1}{|x|^{1+\nu}} \tag{4.36}$$

and in this case the typical parameter ν is defined between 0 and 2 so we have more cases for each value of α. Figure 4.16 shows the different cases studied.

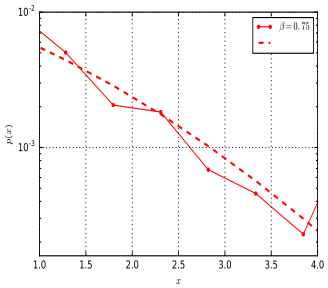
Differently from the previous case the pawer law trend allows us to study in a better way the asymptotic behavior also for the most critical values of ν. Small values of the parameter ν present a slower decay that fits the data in a really good way. For values of ν higher and higher we fall back into the previous problem about values comparable with the numerical errors, especially for small value of α. Note that for $\nu = 1$ we get a *Cauchy* distribution while for ν that tends to 2 we approach the Gaussian pdf.



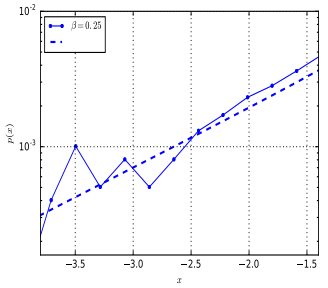
(a) $\alpha = 0.25$.



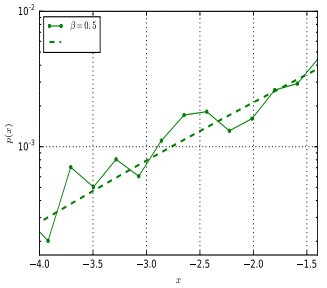
(b) $\alpha = 0.25$.



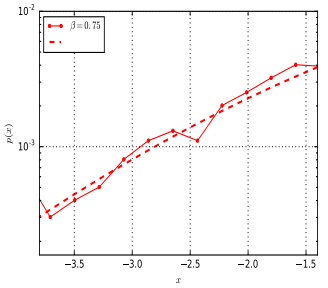
(c) $\alpha = 0.25$.



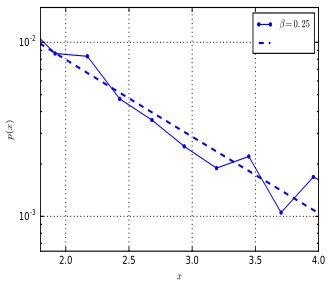
(d) $\alpha = 0.5$.



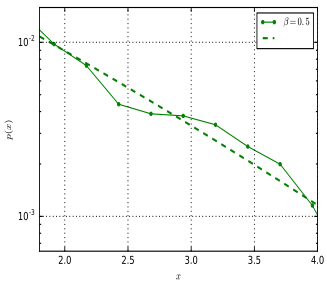
(e) $\alpha = 0.5$.



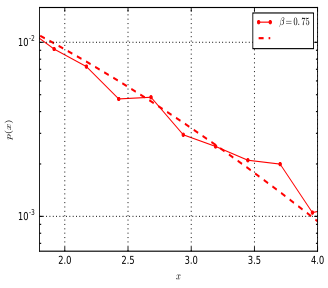
(f) $\alpha = 0.5$.



(g) $\alpha = 0.75$.

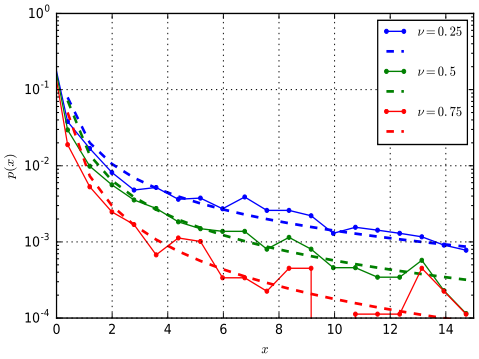


(h) $\alpha = 0.75$.

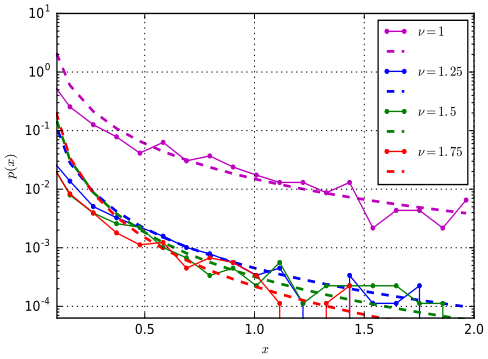


(i) $\alpha = 0.75$.

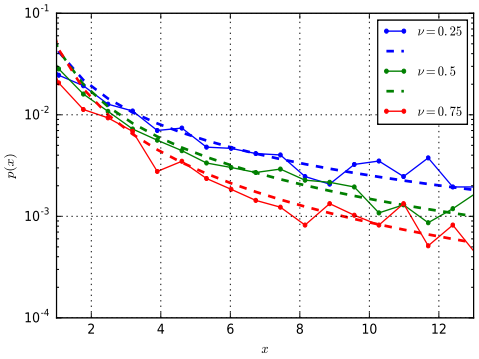
Figure 4.15: Time fractional diffusion: $D_{_V} \sim M_\beta$.



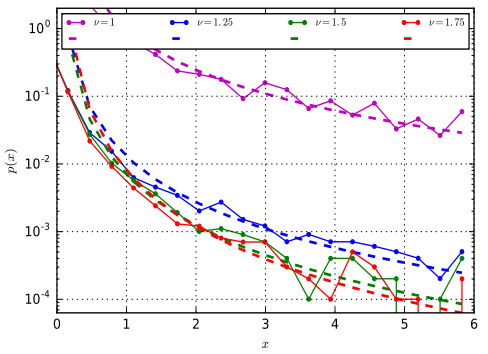
(a) $\alpha = 0.25$.



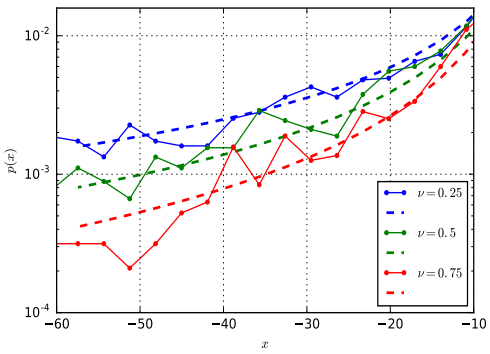
(b) $\alpha = 0.25$.



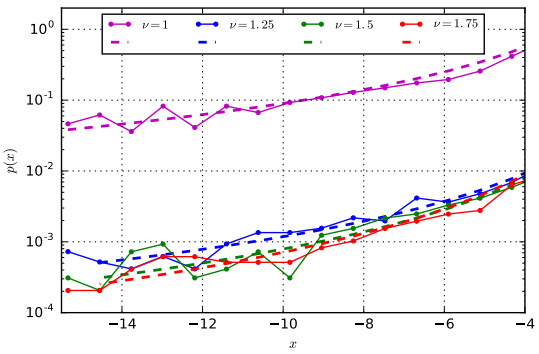
(c) $\alpha = 0.5$.



(d) $\alpha = 0.5$.



(e) $\alpha = 0.75$.



(f) $\alpha = 0.75$.

Figure 4.16: Space fractional diffusion: $D_{_V} \sim L^{EXT}_{\nu/2}$.

Conclusions

The new approach described in Chapter 3 to model fractional diffusion was numerically implemented in this work, considering in particular the superdiffusive case.

We saw how this model, based on a Langevin approach, allows to manage in separate ways the principal features of fractional dynamics: anomalous scaling and non Gaussian pdf. The former is completely monitored by the randomization of the timescale τ while the latter is controlled by the randomization of the velocity diffusivity coefficient $D_{_V}$.

We made use of a random variable generator expressly constructed to generate the suitable distributions for the two random parameters proposed in Chapter 3.

A long tail distribution for the time scale parameter led to difficulties in the choice of the integration scheme for the Langevin equation. As a matter of fact a such large temporal interval for values of τ causes two opposite problems. For really small values of the time scale we need an even smaller temporal step in order to have a serviceable and accurate integration scheme. On the other hand the presence of large value for τ forces the system to need much more time than a standard system to relax; thus, the simulation must be long enough to allow us the observation of the stationary state. Because of these two reasons a scheme with a variable temporal step, which is able to take into consideration the τ variability, was chosen. Furthermore a cut off was realized for values of τ less than 0.004. The numerical error of this scheme was evaluated to be of the order of 10^{-2}.

Once constructed a suitable integration scheme, the check of the expected trends for the position and velocity variances was almost straightforward. It was not the same to test the Gaussianity of the pdfs obtained. In this case the system complexity had not always allow to achieve good results for statistic tests of Gaussianity, especially for the selected integration scheme. Thus, studies on simulations obtained through a fixed temporal step scheme was also introduced to prove the Gaussianity of our samples.

As far as the randomization of $D_{_V}$ is concerned another kind of problem was faced: the absence of an analytical form for the expected pdfs. It prevented the possibility to use statistic tests and so that a study on the asymptotic behavior was realized. The pdf tails sometimes overlapped to the numerical error and thus the fits with the asymptotic behavior were not always extremely precise but both the numerical and the analytical behavior always showed the same trend.

Despite the difficulties above described, due essentially to the complexity of the system, we can conclude that the results obtained in this thesis reproduce the expected anomalous superdiffusive dynamics by means of the new approach here described.

We remember that this approach provides the possibility to deal with the randomization of the parameters in two different steps and it represents a really important factor for two main reasons. First of all it allows to generate a huge variety of stochastic processes, discerning anomalous characteristics from the non Gaussian ones. Secondly, since non Gaussian pdfs emerge when the whole system is considered and not in the single realizations, it allows to reduce the computational efforts that the presence of non Gaussian noise in the simulations had indeed required.

Finally, it is reported that the same path can be retraced to reproduce the subdiffusive case, introducing a harmonic potential into the Langevin equation. The study of subdiffusion through this model is thus let as future research motivated by the promising results achieved in the present thesis.

Appendix

A Fractional derivatives

The *Caputo* time-fractional derivative ${}_tD_*^\beta$ is defined by its Laplace transform as

$$\int_0^{+\infty} e^{-st} \left\{ {}_tD_*^\beta \, u(x;t) \right\} \, dt = s^\beta \, \widetilde{u}(x;s) - \sum_{n=0}^{m-1} s^{\beta-1-n} \, u^{(n)}(x;0^+) \,, \tag{37}$$

with $m-1 < \beta \leq m$ and $m \in N$.

The *Riesz-Feller* space-fractional derivative ${}_xD_\theta^\theta$ is defined by its Fourier transform according to

$$\int_{-\infty}^{+\infty} e^{+i\kappa x} \left\{ {}_xD_\theta^\nu \, u(x;t) \right\} \, dx = -|\kappa|^\nu \, e^{i(sign\kappa)\theta\pi/2} \, \widehat{u}(\kappa;t) \,, \tag{38}$$

with $0 < \nu \leq 2$ and $|\theta| \leq \min \nu, 2-\nu$ as in

In literature the time-fractional derivative is sometimes considered in the *Riemann-Liouville* sense. The relationship of the time-fractional Riemann-Liouville derivative with the time-fractional derivative in the Caputo sense is the following

$${}_tD_*^\beta \, u(x;t) = {}_tD^\beta \, u(x;t) - \frac{t^{-\beta}}{\Gamma(1-\beta)} \, u(x;0) \,. \tag{39}$$

The *Erdélyi-Kober* time-fractional derivative is defined as:

$$D_\eta^{\gamma,\mu} \phi(t) = \prod_{j=1}^{n} \left(\gamma + j + \frac{1}{\eta} t \frac{d}{dt} \right) \left(I_\eta^{\gamma+\mu, n-\mu} \phi(t) \right) , \tag{40}$$

where $n-1 < \mu \leq n$ and $I_\eta^{\gamma,\mu}$ with $\mu > 0$, $\eta > 0$ and $\gamma \in \mathcal{R}$ is the Erdélyi-Kober fractional integral operator given by:

$$I_\eta^{\gamma,\mu} \phi(t) = \frac{t^{-\eta(\mu+\gamma)}}{\Gamma(\mu)} \int_0^t s^{\eta\gamma} (t^\eta - s^\eta)^{\mu-1} \phi(s) d(s^\eta) \,.$$

Also the Erdélyi-Kober time-fractional derivative can be related for a particular case to the Riemann-Liouville derivative through:

$$D_1^{-\mu,\mu} u(x;t) = t^\mu \, {}_tD^\mu u(x;t) \,. \tag{41}$$

B Special functions of fractional calculus

Mainardi fuction

The Mainardi function (ref) $M_\beta(z)$ is defined for every $0 < \beta < 1$ and $\forall\, z \in \mathbb{C}$ by:

$$M_\beta(z) = \sum_{k=0}^{\infty} \frac{(-z)^k}{k!\Gamma\big[-\beta k + (1-\beta)\big]} = \frac{1}{\pi} \sum_{k=0}^{\infty} \frac{(-z)^{k-1}}{(k-1)!} \Gamma(\beta k) \sin(\pi\beta k)\,. \tag{42}$$

This is an entire function of order $\rho = 1/(1-\beta)$ and it provides a generalization of the Gaussian function which can be obtained for $\beta = 1/2$. For our purposes it is useful to consider the main properties of Mainardi function for positive argument $r \geq 0$:

- the Laplace transform is $\mathcal{L}\big\{M_\beta(r/c)\big\} = cE_\beta\big(-cr\beta\big)$, with $c = const$, $\mathbb{R}(s) > 0$ and where $E_\beta(z)$ is the Mittlag-Leffler function;
- in the singular limit of $\beta \to 1^-$ it tends to the Dirac function $\delta(r-1)$;
- the asymptotic representation is

$$\begin{aligned} M_\beta(r) &\sim A_0 Y^{(\beta-1/2)} \exp(-Y)\,, \quad r \to +\infty \\ A_0 &= \frac{1}{\sqrt{2\pi}(1-\beta)^\beta \beta^{(2\beta-1)}}\,, \quad Y = (1-\beta)(\beta^\beta r)^{1/(1-\beta)}\,. \end{aligned} \tag{43}$$

- it can be related to the class of extremal stable distributions by means of

$$M_\beta(r) = \big[L_\beta^{ext}(r)\big]^{-\beta} \tag{44}$$

Lévy stable distributions

The class of α-stable distributions is denoting by $\big\{L_\alpha^\theta(x)\big\}$ with $0 < \alpha \leq 2\,, \theta \leq \min\{\alpha, 2-\alpha\}$. θ represents the skewness parameter and a stable pdf with extremal value for it is defined *extremal*. Stable distributions admit a representation in term of elementary functions only for some particular cases of the parameter values:

1. $\alpha = 2\,, \theta = 0$ *Gauss*:

$$L_2^0(x) = \frac{1}{2\sqrt{\pi}} e^{-x^2/4}, \quad -\infty < x < +\infty\,;$$

2. $\alpha = 1/2\,, \theta = -1/2$ *Lévy-Smirnov*:

$$L_{1/2}^{-1/2}(x) = \frac{x^{-3/2}}{2\sqrt{\pi}} e^{-1/4x}, \quad x \geq 0\,;$$

3. $\alpha = 1\,, \theta = 0$ *Cauchy*:

$$L_1^0(x) = \frac{1}{\pi(x^2+1)}, \quad -\infty < x < +\infty\,.$$

The main characteristics of the stable distributions are:

- they are kind "attractors" for properly normed sums of independent and identically distributed random variables (generalization of the Central Limit Theorem);
- for any value of α the pdfs are unimodal and indeed bell-shaped;
- they fulfill a symmetry relation $L_\alpha^\theta(-x) = L_\alpha^{-\theta}(x)$;
- because of the fat tails they have undefined variance for $\alpha < 2$ and undefined expectation value for $\alpha \leq 1$;
- their characteristic function can be expressed analitically

$$\phi(k) = \begin{cases} \exp\big[-|k|^\alpha \exp(-\frac{\pi}{2} i\theta C(\alpha)\mathrm{sign}(k))\big], & \alpha \neq 1\,, \\ \exp\big[-|k|\big(1 + \frac{2}{\pi} i\theta \ln(k)\mathrm{sign}(k)\big)\big], & \alpha = 1\,, \end{cases}$$

  where $C(\alpha) = 1 - |1-\alpha|$;
- their asymptotic behaviour is defined as $L_\alpha^\theta(x) = O\big(|x|^{-(1+\alpha)}\big), \quad x \to \pm\infty$.

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