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Letter

Minimal model of diffusion with time changing Hurst exponent

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Abstract

We introduce the stochastic process of incremental multifractional Brownian motion (IMFBM), which locally behaves like fractional Brownian motion with a given local Hurst exponent and diffusivity. When these parameters change as function of time the process responds to the evolution gradually: only new increments are governed by the new parameters, while still retaining a power-law dependence on the past of the process. We obtain the mean squared displacement and correlations of IMFBM which are given by elementary formulas. We also provide a comparison with simulations and introduce estimation methods for IMFBM. This mathematically simple process is useful in the description of anomalous diffusion dynamics in changing environments, e.g. in viscoelastic systems, or when an actively moving particle changes its degree of persistence or its mobility.

Supplementary material for this article is available online

Keywords: diffusion, long-range correlations, fractional Brownian motion (Some figures may appear in colour only in the online journal)

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1. Introduction and background

The modern study of diffusive processes started at the beginning of the 20th century when Albert Einstein [1], Marian Smoluchowski [2], William Sutherland [3], and Paul Langevin [4] proposed the physical theory of Brownian motions (later formalized by Norbert Wiener [5]), laying the foundations for what is now the theory of stochastic processes and nonequilibrium statistical physics [6–9]. Brownian motion is characterized by a linear mean squared displacement (MSD) and a Gaussian probability density function (PDF) [10, 11]. While single particle tracking already was well established in the early experiments of Perrin [12] and Nordlund [13], with modern microscopic techniques the stochastic motion of microscopic particles or even single molecules can now be routinely recorded in complex environments such as living biological cells [14]. Single trajectories are also measured for moving cells, small organism, or even large animals, among many other applications [14–20]. Such experiments demonstrate that in many complex systems the MSD is no longer linear in time but follows the power-law form $\langle X^2(t)\rangle \propto t^{2H}$, where the Hurst exponent H distinguishes subdiffusion (0 < H < 1/2) from superdiffusion (1/2 < H < 1) [21].

A widely used generalization of the Einstein–Smoluchowski–Langevin theory of Brownian motion is fractional Brownian motion (FBM) $B_H(t)$, the only stochastic process which is Gaussian and exhibits power-law memory between its increments⁴

$$\left\langle \frac{\mathrm{d}B_H(s)}{\mathrm{d}s} \frac{\mathrm{d}B_H(t)}{\mathrm{d}t} \right\rangle = DC_H|t - s|^{2H - 2}, \quad C_H \equiv H(2H - 1). \tag{1}$$

Here the parameter D is the (generalized) diffusion coefficient. Integrating over this formula twice shows that the MSD has the power-law form $\langle B_H(t)^2 \rangle = Dt^{2H}$. In this context the coefficient D can be interpreted as the scale of the process for a given anomalous diffusion exponent 2H. A process closely related to FBM was originally proposed by Kolmogorov [23], and FBM was widely popularized by Benoît Mandelbrot and John van Ness in their seminal paper [24, 25]. Mandelbrot and van Ness were in fact inspired not by diffusion, but Harold Hurst's studies of water flows [26], economic cycles, and fractional $1/f^{\alpha}$ noises. In line with their interdisciplinary approach, contemporary applications of FBM span very diverse fields, from broadband network traffic [27] to the structure of star clusters [28], and financial market dynamics [29]. Characteristics of subdiffusive FBM were, i.a., observed for the motion of submicron tracers in soft and bio matter [30–36]. Superdiffusive motion consistent with FBM was observed in actively driven motion in biological cells [37, 38] and in movement ecology [15, 39]. We note that non-Gaussian forms of FBM measured, e.g. in biological cells [40–42], may arise from FBM with randomly fluctuating diffusion coefficient [43–46].

The cases of subdiffusion (0 < H < 1/2) and superdiffusion (1/2 < H < 1) have differing physical interpretations and are only rarely observed together [36, 47]. For 0 < H < 1/2 the process exhibits negative memory (see equation (1)), a property referred to as antipersistence. The negative dependence between increments and the covariance integrates to zero, $\int_{-\infty}^{\infty} \left\langle \frac{\mathrm{d}B_H(s)}{\mathrm{d}s} \frac{\mathrm{d}B_H(s+t)}{\mathrm{d}t} \right\rangle \mathrm{d}t = 0.$ For 1/2 < H < 1 the positive dependence between increments

⁴ For $H \le 1/2$ this expression has a strong singularity at $t - s = w \to 0$ which should be carefully accounted for. In integrals it is interpreted as $\frac{d}{dw}(H|w|^{2H-1}\operatorname{sgn} w)$ [22], similarly to equation (3) below.



causes the memory to be persistent, featuring a non-integrable tail of the covariance function, such that $\int_1^\infty \langle \frac{\mathrm{d} B_H(s)}{\mathrm{d} s} \frac{\mathrm{d} B_H(s+t)}{\mathrm{d} t} \rangle \mathrm{d} t = \infty$ [48]. It is worth adding that FBM is also used as a noise in generalized Langevin equations [49–51].

Definition (1), while uniquely determining FBM and separating it from other anomalous diffusion models, such as non-Gaussian subdiffusive random walks [21], does not provide an explicit construction of the FBM process. This can be achieved with one of the few equivalent integral representations. The Fourier representation, equivalently for the increments and the process itself, reads⁵

$$dB_{H}(t) = \frac{\sqrt{D}}{\gamma_{H}} \int_{-\infty}^{\infty} \frac{i\omega e^{i\omega t}}{|\omega|^{H+1/2}} dt dZ(\omega) \quad \text{and} \quad B_{H}(t) = \frac{\sqrt{D}}{\gamma_{H}} \int_{-\infty}^{\infty} \frac{e^{i\omega t} - 1}{|\omega|^{H+1/2}} dZ(\omega)$$
 (2)

with the rescaling constant $\gamma_H \equiv \sqrt{2\pi}(\sin(\pi H)\Gamma(2H+1))^{-1/2}$. This representation has the advantage of emphasizing that FBM is a model for a system at statistical equilibrium. Indeed, shifting time by some t_0 only multiplies the integrand on the left by the complex phase $\exp(it_0\omega)$ which leads to the same (real valued) PDF due to Gaussian distribution isotropy of the dZ. It also directly demonstrates that FBM is a $1/f^{\alpha}$ process with power spectral density $|\omega|^{1/2-H}$. Another representation of FBM is the integral $\int_{-\infty}^{t} \left((t-s)_+^{H-1/2} - (-s)_+^{H-1/2}\right) dB_s$ with $(t)_+ \equiv \max(t,0)$; for more details see [52].

The strong symmetries of FBM make its Hurst index the unifying parameter governing both its short and long time properties. This fact restricts some of its applications—crucially for us it makes it impossible to describe an increasing number of regime-switching anomalous diffusion systems in which the anomalous diffusion exponent and the diffusivity change as functions of time. Examples for such phenomena include the motion of a tracer in the changing viscoelastic environment of cells during their cycle [53] or in viscoelastic solutions under pressure and/or concentration changes [54, 55], in actin gels with changing mesh size [56], the motion of lipid molecules in cooling bilayer membranes [35], passive and active intracellular movement after treatment with chemicals [37, 57], or intra- and inter-daily variations in the movement dynamics of larger animals [58]. Quite abrupt changes of *H* and/or *D* may be effected by binding to larger objects or surfaces [41, 59] or multimerization [59, 60] of the tracer.

In order to overcome the limitations of FBM, multifractional Brownian motion (MFBM) models were created, initially motivated by terrain modeling [61]. A process is considered to be an MFBM if it resembles FBM locally, i.e. its increments dX(t) resemble increments of FBM dB_H with local parameters, a property called local self similarity [62]. This definition does not specify any global features of the process, such as the dependence between different dX(s) and dX(t)—these can vary from model to model. Benassi, Roux and Jaffard proposed an especially useful MFBM defined by substituting $H \to \mathcal{H}_t$ into the right hand side of the integral in equation (2) [63]. The simple mathematical form of the Fourier transform allowed Ayache *et al* to calculate the exact distribution of this model, a clear advantage for practical applications; in particular it has MSD $Dt^{2\mathcal{H}_t}$ [64]. For information about other MFBM variants see, e.g. the

⁵ Mathematically interpreted as the stochastic integral over complex-valued white Gaussian noise $dZ(\omega)$.



2006 review by Stoev and Taqqu [65]. Recently, a memory MFBM (MMFBM) model was proposed in order to describe viscoelastic or persistent anomalous diffusion with physically meaningful persistence of correlations [66]. Another very closely related class of processes are linear time series models with fractionally integrated noises (ARFIMA) and time dependent coefficients [67]. Inter alia MFBMs found applications in finance, where it is natural to expect a time-dependence of the market dynamics [68–71], and also network traffic [72], geometry of mountain ranges [73] or atmospheric turbulence [74], as well as heterogeneous diffusion [45]. Statistical methods for analyzing MFBM models include wavelet decomposition [75], covariance and MSD analysis and testing [76], or neural networks [77].

In the standard MFBM models the history of the Hurst exponent \mathcal{H}_s , s < t does not affect future observed displacements, only the local value of \mathcal{H}_t matters. This feature does not affect the above-mentioned applications of MFBMs as they are mostly concerned with the local roughness of the observed data, not its global moments and correlations. This 'amnesia' of the Hurst exponent is also the reason behind MFBMs' simple mathematical structure. However, it is not a desirable property for modeling diffusion in complex media where an evolving \mathcal{H}_t should reflect the physical changes in the environment which determine the further evolution of the process due to the inherent long-range memory. The forgetfulness of MFBMs also forces the trajectories to 'bend' to an evolving \mathcal{H}_t : Rapid changes of \mathcal{H}_t lead to rapid, jump-like changes of the trajectory X(t). In physical and biological contexts we would rather expect that—in the same manner as for the diffusivity—changes of H (even rapid) should lead to a gradual response to a new environment due to the governing long-range memory structure.

In the following we introduce and state the fundamental properties of a minimal model for FBM with a time-evolving Hurst exponent in section 2. We then present concrete results for a step-wise change of the Hurst exponent and the diffusion coefficient in section 3. Finally we discuss our results in a broader context in section 4. Simulation and estimation methods for the model are shown in the supplementary material.

2. Definition of the minimal model

In our approach to establish a minimal model to resolve the question of how we can model anomalous diffusion of the FBM type with long-range correlations and time-evolving transport coefficients H and D we want to preserve the simple mathematical structure of the existing MFBM models but modify this structure such that it does not directly affect the position of the particle but reflects the gradual influence on the particle dynamics following environmental changes as mediated by the memory structure of FBM. To this end we consider an FBM-type diffusion for which the change in the environment leads to changes of the Hurst exponent and diffusion coefficient. It is then physically more natural to assume that this will not cause the whole trajectory to 'switch' to a new H, but only affect the new increments after the change. In different words, changes of H should lead to direct changes of the increments and to only indirect changes of the position.

The simplest way of fulfilling this requirement is to modify the memory structure of FBM to

$$\left\langle \frac{\mathrm{d}B_{\mathcal{H}}(s)}{\mathrm{d}s} \frac{\mathrm{d}B_{\mathcal{H}}(t)}{\mathrm{d}t} \right\rangle = \sqrt{\mathcal{D}_s \mathcal{D}_t} C_{\mathcal{H}_s, \mathcal{H}_t} |t - s|^{\mathcal{H}_s + \mathcal{H}_t - 2}, \tag{3}$$



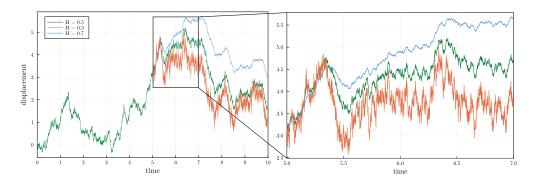


Figure 1. Comparison of three trajectories, which represent normal Brownian motion until t=5 and then switch to subdiffusion, superdiffusion, or stay Brownian. The trajectories are based on the same realization of the stochastic noise. We see how a low H(<1/2) introduces antipersistence by amplifying the periods in which the trajectory turns back and, conversely, how high H(>1/2) introduces a persistence by amplifying excursions in the same direction. The right panel shows a zoom into the part of the trajectory right after the switching of H. The simulations were performed using our introduced model with time changing H, the procedure is explained in the supplementary material.

where the rescaling constant $C_{\mathcal{H}_s,\mathcal{H}_t}$ ($C_{H,H}=C_H$) is to be determined at the end of this section. We also require the process to be Gaussian, as is FBM. Thus, the process (3) is uniquely determined, as there is only one Gaussian variable with a given covariance (and zero mean). The resulting dynamic has a Hurst index defined by the arithmetic mean $H \to (\mathcal{H}_s + \mathcal{H}_t)/2$ and a diffusion coefficient given by the geometric mean $D \to \sqrt{\mathcal{D}_s \mathcal{D}_t}$. For any period with constant parameters $\mathcal{H}_t = H$ and $\mathcal{D}_t = D$ this process clearly reduces to a standard FBM, and thus this process belongs to the broad class of MFBMs. As it is defined through its increments we will call it incremental MFBM (IMFBM). We demonstrate how a changing Hurst exponent affects IMFBM trajectories in figure 1. We note that the trajectory of MBFM would lead to a discontinuity at the point where H is changing.

Equation (3) completely determines the memory structure of IMFBM. The quantity $\langle dB_{\mathcal{H}}(s)dB_{\mathcal{H}}(t)\rangle$ can be interpreted as a response function r=r(s,t), that determines to which extent any past infinitesimal change $dB_{\mathcal{H}}(s)$ influences linearly the current change $dB_{\mathcal{H}}(t)$: the feedback is negative, i.e. r<0, for $\mathcal{H}_s+\mathcal{H}_t<1$ and positive (r>0) for $\mathcal{H}_s+\mathcal{H}_t>1$. A heavy, non-integrable tail of r is present when $\mathcal{H}_s+\mathcal{H}_t>1$.

Assuming we start our observation at 0, $B_{\mathcal{H}}(0) = 0$, the MSD of IMFBM can be obtained from the integral⁶

$$\langle B_{\mathcal{H}}(t)^{2} \rangle = \left\langle \left(\int_{0}^{t} dB_{\mathcal{H}}(s) \right)^{2} \right\rangle = \int_{0}^{t} \int_{0}^{t} \langle dB_{\mathcal{H}}(s_{1}) dB_{\mathcal{H}}(s_{2}) \rangle, \tag{4}$$

where the integrand is given by relation (3). Analogously, to obtain the full covariance $\langle B_{\mathcal{H}}(s)B_{\mathcal{H}}(t)\rangle$ only the limits of the integrals are changed to $\int_0^s \int_0^t$. Note that the result does

⁶ This formulation is connected to Riemman Liouville FBM as originally formulated by Lévy [24, 78].



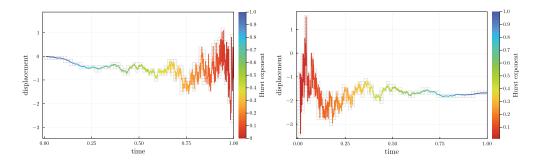


Figure 2. Trajectory of IMFBM for which the Hurst exponent decreases linearly from 1 to 0 (left panel) or increases linearly from 0 to 1 (right panel). The grey areas show boxes with fixed size ϵ , which cover the trajectory. The more irregular the trajectory is locally, the more it 'covers' the space. In the limit $\epsilon \to 0$ the number of required boxes locally increases proportionally to the fractal dimension, $\epsilon^{-(2-\mathcal{H}_t)}$ [82].

not depend on the past of $\mathcal{H}_t, \mathcal{D}_t, t < 0$. If the evolution of the system initiated at some $t_0 < 0$ and we started observing it at time t = 0 the measured displacements $B_{\mathcal{H}}(t) - B_{\mathcal{H}}(0)$ would be the same as in (4). This is a practical feature based on the stationarity, ingrained in (3), of the underlying displacements, due to which IMFBM depends only on observed quantities.

From equation (4) it is also apparent that in the special case $\mathcal{H}_t = H = \text{const.}$ and $\mathcal{D}_t \neq \text{const.}$ the process reduces to

$$B_{\mathcal{H}}(t) = \int_0^t \sqrt{\mathcal{D}_s} dB_H(s), \tag{5}$$

which is a natural choice of extending FBM to incorporate a time-varying diffusivity [66]. When $\mathcal{H}_t = 1/2$ this integral reduces to scaled Brownian motion, a widely used Markovian model of diffusion with time-evolving diffusivity [79, 80].

The above example shows that the choice of time changing diffusivity $D \to \sqrt{\mathcal{D}_s \mathcal{D}_t}$ appears quite natural. The second part of the IMFBM definition, the choice of $H \to (\mathcal{H}_s + \mathcal{H}_t)/2$ can be interpreted as imposing a linear dependence on the Hurst exponent history. The current increment $dB_{\mathcal{H}}$ is correlated with a past increment with a weight proportional to $|t-s|^{\mathcal{H}_s}ds$. This relation is linear only for substitutions of the form $H \to \lambda \mathcal{H}_s + (1-\lambda)\mathcal{H}_t$ with $0 \le \lambda \le 1$. Giving equal weight to past and present, $\lambda = 1/2$, appears as a reasonable default choice. It also makes sure that trajectories of IMFBM (analogously to other MFBMs) locally resemble FBM with parameters $\mathcal{D}_t, \mathcal{H}_t$, thus preserving the local roughness of the trajectory: for smooth changes of \mathcal{H} and \mathcal{D} it has local fractal dimension $2 - \mathcal{H}_t$, 7 as illustrated in figure 2.

Returning to equation (3), we note that similar to (1) for FBM, it does not provide a representation (a direct construction) of the process. In fact, without such a representation, one cannot even be sure that such a process exists mathematically. Due to its elegant mathematical

⁷ It fulfils the conditions for a fractal dimension given in [81].



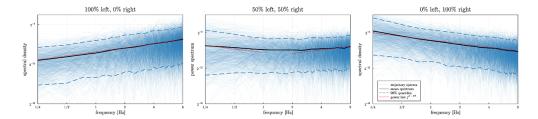


Figure 3. Spectral densities calculated from a window of 1000 differentiated IMFBM trajectory realizations with a single change of parameters from $H_1 = 0.3$, $D_1 = 1$ to $H_2 = 0.7$, $D_2 = 16$ (see also section 3). In the Left panel the window is fully in the range of $H_1 = 0.3$ and the power law spectrum agrees with the one of classical FBM. In the Right panel, analogously, we see the same for a window fully in the range of $H_2 = 0.7$. In the Centre panel we observe a mixed spectrum which on the left side is mostly affected by the subdiffusive $H_1 = 0.3$ and on the right by the superdiffusive $H_2 = 0.7$.

form the Fourier definition (2) of FBM turns out to be useful here, as well. We simply substitute $D \to \mathcal{D}_t$ and $H \to \mathcal{H}_t$ into the left integral in (2) and get⁸

$$dB_{\mathcal{H}}(t) \equiv \frac{\sqrt{\mathcal{D}_t}}{\gamma_{\mathcal{H}_t}} \int_{-\infty}^{\infty} \frac{i\omega e^{i\omega t}}{|\omega|^{\mathcal{H}_t + 1/2}} dt \, dZ(\omega). \tag{6}$$

By construction, this representation makes sure that the process is Gaussian, as a combination of Gaussian increments $dZ(\omega)$. For $\mathcal{H}_t, \mathcal{D}_t \neq \text{const.}$ the process is non-ergodic and nonstationary. Its increments belong to the class of evolutionary spectra processes [83] with powerlaw time dependent spectrum $\text{sgn}(\omega)|\omega|^{1-2\mathcal{H}_t}$, see figure 3. This power-law distribution of the probability mass over frequencies determines the local fractal properties of the process, which are locally like those of regular FBM.

It follows from the linearity of the Fourier transform that the covariance of IFBM fits our requirement (3); essentially this process has the two-point Fourier amplitude $\propto \sqrt{\mathcal{D}_s \mathcal{D}_t} |\omega|^{1-\mathcal{H}_s-\mathcal{H}_t}$ and it enforces (3). Using relation (6) we can determine the rescaling coefficient $C_{\mathcal{H}_s,\mathcal{H}_t}$: this can be achieved using integral tables from which we find $C_{\mathcal{H}_s,\mathcal{H}_t} = c_{\mathcal{H}_s,\mathcal{H}_t} C_{(\mathcal{H}_s+\mathcal{H}_t)/2}$ with $c_{\mathcal{H}_s,\mathcal{H}_t} \equiv \gamma_{(\mathcal{H}_s+\mathcal{H}_t)/2}^2/(\gamma_{\mathcal{H}_s}\gamma_{\mathcal{H}_t})$. For periods of constant H, $c_{H,H} = 1$, $c_{H,H} = c_{H}$; otherwise the ratio c weakens the dependence by a factor increasing with the difference between \mathcal{H} values which accounts for the varying local amplitudes of different trajectory segments.

3. Stepwise changes of Hurst exponent and diffusion coefficient

The simplest—and essential—practical example for an evolving H concerns the switching between one distinct type of environment to another, and for which we can neglect the influence of short transition periods. In the model we then have that $\mathcal{H}_t, \mathcal{D}_t$ reduce to step functions with values (H_1, D_1) , (H_2, D_2) , etc at fixed intervals. As in any of the intervals with constant $\mathcal{H}_t, \mathcal{D}_t$ the increments of IMFBM are—in isolation—equivalent to FBM increments,

⁸ The process here is understood as a random generalized function, i.e. this definition uniquely determines all integrals $\int \phi(t) dB_{\mathcal{H}}(t)$ for bounded ϕ with bounded support.



the corresponding pieces of trajectory are identical to segments of FBM with corresponding parameters H_j, D_j . If such a segment were measured without the rest of the trajectory the *increments* would be indistinguishable from those of normal FBM. Any statistical property, based on ensemble-averages, time-averages, or both, will be the same. When multiple such segments are experimentally observed, the IMFBM model provides additional information about their codependence on the level of the *position*. Namely, any two trajectory segments depend on each other through their compound Hurst exponents and diffusivities, $(H_j + H_{j+1})/2$ and diffusivity $c_{H_j,H_{j+1}} \sqrt{D_j D_{j+1}}$. Additionally, the full memory structure of a trajectory $B_{\mathcal{H}}$ for any number of transitions can be expressed by the direct formula obtained from the covariance integral (4), see equation (S3).

To better understand the behavior of this model let us consider a simple concrete case crucial for many applications. A single transition between two pairs of values (H_i, D_i) at time τ corresponds to the protocol

$$\mathcal{H}_t = \begin{cases} H_1, & t \leqslant \tau, \\ H_2, & t > \tau, \end{cases} \qquad \mathcal{D}_t = \begin{cases} D_1, & t \leqslant \tau, \\ D_2, & t > \tau. \end{cases}$$
 (7)

The associated MSD reads

$$\langle B_{\mathcal{H}}(t)^{2} \rangle = \begin{cases} D_{1}t^{2H_{1}}, & t \leq \tau, \\ D_{2}(t-\tau)^{2H_{2}} + D_{1}\tau^{2H_{1}} \\ +c_{H_{1},H_{2}}\sqrt{D_{1}D_{2}} \left(t^{H_{1}+H_{2}} - (t-\tau)^{H_{1}+H_{2}} - \tau^{H_{1}+H_{2}}\right), & t > \tau. \end{cases}$$
(8)

The cross term for $t > \tau$ has the asymptotic $\sim (H_1 + H_2)\tau c_{H_1,H_2}\sqrt{D_1D_2}t^{H_1+H_2-1}$. Thus, as expected, the MSD is dominated by H_2 at long times, $\langle B_{\mathcal{H}}(t)^2 \rangle \sim D_2 t^{2H_2}$, $t \to \infty$. When $H_1 + H_2 < 1$ the cross term disappears completely at long times. In the opposite regime $H_1 + H_2 > 1$ its remaining presence is indicative of the long memory in the system. Shortly after the transition at, $t = \tau + \delta$ with $\delta \to 0$, the asymptotic expansion of the MSD reads

$$\langle B_{\mathcal{H}}(t)^2 \rangle \sim D_1 \tau^{2H_1} + D_2 \delta^{2H_2} + (H_1 + H_2) c_{H_1, H_2} \sqrt{D_1 D_2} \tau^{H_1 + H_2 - 1} \delta - c_{H_1, H_2} \sqrt{D_1 D_2} \delta^{H_1 + H_2}.$$
(9)

Among the three terms depending on δ the one with the smallest exponent dominates at $\delta \to 0$. Interestingly, in the case of weakening subdiffusion $H_1 + H_2 < 1$, $H_1 < H_2$, or subdiffusion with decreasing diffusivity $H_1 = H_2 < 1/2$, $D_2 < D_1$, after the transition at τ the MSD locally decreases. This may at first be seen as a paradox, taking into account that displacements after time τ do increase, $\langle (B_{\mathcal{H}}(t+\tau) - B_{\mathcal{H}}(\tau))^2 \rangle = D_2 t^{2H_2}$. However, a similar behavior can also be observed for other models with time-dependent antipersistence and is caused by the fact that locally antipersistence dominates persistence, $t^{2H_1} \ll t^{2H_2}$ for $H_2 < H_1, t \to 0$. Thus, the tendency to reverse the progression wins until a new piece of trajectory accumulates sufficient weight. The same effect occurs for decreasing D as then new increments have less weight due to their smaller amplitudes. Different examples of Hurst exponent transitions are shown in figure 4.



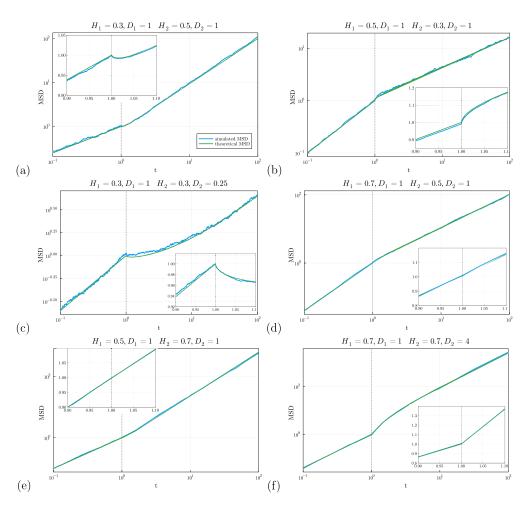


Figure 4. Illustration of different types of transitions at t = 1: (a) subdiffusion to normal diffusion, (b) normal to subdiffusion, (c) subdiffusion to subdiffusion with different diffusivity, (d) superdiffusion to normal diffusion, (e) normal diffusion to superdiffusion, and (f) superdiffusion to superdiffusion with different diffusivity. The MSDs in the main plots were estimated using 10^3 trajectories. In order to visualize details of the motion, in the inset plots with larger samples of 10^5 were used.

4. Discussion

The subject of anomalous diffusion is sometimes called a 'jungle' of models which alludes to the richness and variety of mathematical tools it offers but also to common difficulties in deciphering the ones best suited to a given system. New methods of describing transient diffusion phenomena introduce additional time dependencies of the transport parameters which adds yet another layer to the already complex modeling problem. This is why it is crucial to have at disposal models as simple as possible, and which preserve as much as possible from the elegant symmetries of anomalous diffusion processes—this is what made them useful in the first place.



Table 1. Comparison of typical already established MFBM models and IMFBM for one change of Hurst exponent at time τ . In the line for MSD $H_* \equiv \min\{H_2, 1/2, (H_1 + H_2)/2\}$ and constant D_* can be read from the full formula (8). Note that for different variants of MFBM the exact behavior in the left column my differ, the features given are typical, see [65].

	Classical MFBMs	IMFBM
Dependence	Long memory	Long memory
Fractal dimension	$\begin{cases} 2 - H_1, & t < \tau \\ 2 - H_2, & t > \tau \end{cases}$	$\begin{cases} 2 - H_1, & t < \tau \\ 2 - H_2, & t > \tau \end{cases}$
MSD	$\begin{cases} Dt^{2H_1}, & t \leqslant \tau \\ Dt^{2H_2}, & t > \tau \end{cases}$	$\begin{cases} D_1 t^{2H_1}, & t \leq \tau \\ \sim D_1 \tau^{2H_1} + D_* (t - \tau)^{2H_*}, & t > \tau \end{cases}$
Trajectories	Discontinuous at τ	Continuous

What is presented here is an attempt at introducing a time dependence into FBM while keeping its memory structure as simple as possible. Such processes—MFBMs—have already been developed but they were not widely used for describing diffusion phenomena and existing models do not have probabilistic features which we would expect from those for physical and biological systems. The introduced IMFBM models a particle diffusing in a complex environment for which conditions change in time and after the transition new displacements are governed by new diffusivity and new Hurst exponent while also keeping the memory of its history before the transition; see table 1 for a comparison between classical MFBM models and IFBM. It has two central features: the geometric averaging of diffusivities and arithmetic averaging of Hurst exponents (see (3)) which are fully experimentally verifiable and distinguish it from other MFBM models.

IMFBM is a generalization of both FBM and scaled Brownian motion used to model diffusion with changing diffusivity. The transitions of H and D can be both smooth or discontinuous. It is Gaussian. The associated MSD and covariance can always be expressed as integrals which for the crucial case of step function protocols for H and D reduce to elementary functions. The local fractal dimension of the IMFBM trajectories is $2 - \mathcal{H}_t$.

Mathematical models such as IMFBM are indispensable in creating objective tools to determine the best combination of stochastic models and their parameters given measured data. They are becoming increasingly important with the fast growing numbers of increasingly refined experiments in complex systems. Some of the existing solutions are provided, e.g. by Bayesian analyzes [84, 85] or the machine learning apparatus [20, 86–88]. We provide a guide towards statistical estimation of the transport parameters in our IMFBM model in the supplementary material.

The IMFBM process can be used to model the data directly but we also see a potential value in using it to construct more sophisticated tools. In many systems the evolution of H and D should be considered to be random itself. This is an example of a doubly stochastic modeling approach which is straightforward to introduce into anomalous diffusion studies using IMFBM. Another classical and indispensable tool in stochastic modeling are Langevin equations which are a class of stochastic differential equations suited to describe the diffusion phenomena. It seems very natural to use IMFBM as a noise in those equations which would then allow us to study the stochastic motion in the presence of an external potential and which fulfills local fluctuation—dissipation relations.



Data availability statement

No new data were created or analysed in this study.

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