Local evolution equations for non-Markovian processes

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Abstract

A Fokker-Planck equation approach for the treatment of non-Markovian stochastic processes is proposed. The approach is based on the introduction of fictitious trajectories sharing with the real ones their local structure and initial conditions. Different statistical quantities are generated by different construction rules for the trajectories, which coincide only in the Markovian case. The merits and limitations of the approach are discussed and applications to transport in ratchets and to anomalous diffusion are illustrated.

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Anomalous behaviours in the fluctuations of physical quantities are a common occurrence, typically associated with lack of separation between the macroscopic and the fluctuation scale [1]. An important example is transport in complex systems such as disordered media [2], colloidal suspensions [3] and turbulent flows [4]. If a scale separation were present, the system could be described by a local fluctuation-dissipation process, which could be expressed as a stochastic differential equation of the standard Langevin type. The short-time dynamics of the fluctuating variable, call it \( Y \), would then be characterized by normal diffusion, and there would exist local Fokker-Planck and backward Kolmogorov equations, describing the dynamics of the transition PDF (probability density function) \( \rho(Y, t|Y_0, t_0) \) [5].

In general, anomalous behaviours could not be accounted for by a stochastic differential equation and the non-Markovian nature of the process would be associated with equations for the PDF, which are of integro-differential (fractional) form in time [6]. This implies that, in general, the evaluation of statistical quantities will require dealing with memory kernels in the equation for \( Y \) and with the effect of aging [7]. However, as we shall discuss in this letter, there are situations in which a description of the PDF dynamics, not requiring the use of fractional equations, becomes possible.

Imagine to evaluate the average at time \( t_2 \) of some function of \( Y \), given the initial condition \( Y(t_0) = Y_0 \). Hence, we are going to need the transition PDF \( \rho(2|0) \) (we are going to use the shorthand \( k \) to indicate the pair \( Y_k, t_k \)). Suppose we have already evaluated \( \rho(1|0) \) for \( t_0 < t_1 = t_2 - \Delta t \) and we want to propagate \( \rho(1|0) \) to \( \rho(2|0) \). Then, the following relation holds:

\[
\rho(2|0) = \int \! dY_1 \rho(2|1; 0) \rho(1|0)
\] (1)

which, in the case of a Markovian process, for which \( \rho(2|1; 0) \rightarrow \rho(2|1) \), turns into a standard Chapman-Kolmogorov equation.

This relation could be generalized to statistical conditions at \( n \neq 1 \) times. In particular, the case \( n = 0 \) is realized by a standard Chapman-Kolmogorov equation in which the propagating kernel is \( \rho(2|1) \). Similarly, it is possible to consider joint PDF’s in the form \( \rho(1|0) \), \( \mathbf{1} = \{1, 1', \ldots\} \), \( \mathbf{0} = \{0, 0', \ldots\} \) and Eq. [11] would read:

\[
\rho(2|0) = \int \! dY_1 \rho(2|1; 0) \rho(1|0).
\] (2)
Hence, contrary to the Markov case, generalized Chapman-Kolmogorov equations propagating PDF's with different conditionings at times \( t_0, t'_0, \ldots \) involve different transition kernels \( \rho(2|1; 0) \).

A physical interpretation of this multiplicity is obtained observing that an equation like (1) describes the evolution of fictitious trajectories \( \tilde{Y}(t) \) obeying an equation in the form
\[
\tilde{Y}(t_2) = \tilde{Y}(t_1) + \mathcal{\langle} \Delta Y|1; 0 \mathcal{\rangle} + \Delta W
\] (3)
with initial condition given by the pair \( Y_0, Y_1, t_1 - t_0 \to 0 \). In this equation, \( \Delta Y = Y(t_2|1; 0) - \tilde{Y}(t_1) \) and \( \Delta W \) has zero mean and statistics determined, in the \( \Delta t \to 0 \) limit, by \( \mathcal{\langle} \Delta W^2|1; 0 \mathcal{\rangle} \). These trajectories are fictitious in the sense that they are not typical realizations of the process \( Y \). In fact, in the case of a real trajectory, \( \tilde{Y}(t_2) \) would be obtained from \( Y(t_1) \) using informations on the whole history before \( t_1 \), and not only at \( t = t_0 \) or, in the case of Eq. (2), at the discrete instants \( t_0, t'_0, \ldots \) Only in the Markov case, cease the trajectories to be fictitious and become typical realizations of the process, coincident in form for different \( n \). This in analogy with Eq. (1), which, in the Markov case, takes the unique standard Chapman-Kolmogorov form.

It is possible to introduce a Fokker-Planck formalism to describe the evolution of the 1-time statistics for the fictitious trajectories and hence of the PDF \( \rho(Y, t|Y_0, t_0) \). To understand the form of the Fokker Planck equation associated with Eq. (1), consider the case of a Gaussian stationary process with generic power law scaling at small time separations: \( C(t) = \mathcal{\langle} Y(\tau)Y(\tau + t) \mathcal{\rangle} \sim \sigma^2 - B|t|^\alpha /2, |t| \ll (\sigma^2/B)^{1/\alpha} \). [This process can be turned into a fractional Brownian motion sending \( \sigma \to \infty \) and allowing \( C(t) = \sigma^2 - B|t|^\alpha /2 \) for generic \( t \). In the case of a Gaussian process, explicit expressions for \( \mathcal{\langle} \Delta Y|1; 0 \mathcal{\rangle} \) and \( \mathcal{\langle} \Delta W^2|1; 0 \mathcal{\rangle} \) can be obtained analytically (3):
\[
\begin{align*}
\mathcal{\langle} \Delta Y|1; 0 \mathcal{\rangle} &= \sum_{lm=0}^{1} C_{2l} D_{lm} Y_m - Y_1 \\
\mathcal{\langle} \Delta W^2|1; 0 \mathcal{\rangle} &= C_{22} - \sum_{lm=0}^{1} C_{2l} D_{lm} C_{m2}
\end{align*}
\] (4)
where \( C_{ij} = \mathcal{\langle} Y(t_i)Y(t_j) \mathcal{\rangle} \) is the correlation matrix at instants \( t_k, k = 0, 1, 2 \) and \( D_{ij} \) is the inverse of its restriction to \( k = 0, 1 \): \( \sum_{j=0}^{1} D_{ij} C_{jk} = \sum_{j=0}^{1} C_{ij} D_{jk} = \delta_{ik} \).

In this way we have, for \( t_2 = t_1 + dt \) and \( t_1 = t_0 + t \), with \( t \) generic: \( C_{kk} = \sigma^2, k = 0, 1, 2 \), \( C_{01} = C_{10} = C(t) \), \( C_{12} = C_{21} = \sigma^2 - Bdt^\alpha /2 \) and \( C_{02} = C_{20} = C(t) + C'(t)dt \). Similarly for \( D_{ij} \): \( D_{00} = D_{11} = \sigma^2 \Phi(t) \) and \( D_{01} = D_{10} = -\Phi(t)C(t) \), where \( \Phi(t) = [\sigma^4 - C^2(t)]^{-1} \).
Substituting into Eq. (4), we find:

\[ \langle dW^2 | 1; 0 \rangle = B dt^\alpha \]

and

\[ \langle dY | 1; 0 \rangle = \Phi(t) \left\{ \left[ -\sigma^2 B dt^\alpha / 2 - C(t)C'(t) dt \right] Y_1 
+ \left[ BC(t) dt^\alpha / 2 + \sigma^2 C'(t) dt \right] Y_0 \right\} \]

(6)

Similar calculations could be performed also for \( \langle dW^2 | 1 \rangle \) and \( \langle dY | 1 \rangle \) and the result is:

\[ \langle dW^2 | 1 \rangle = -\sigma^2 Y_1^{-1} \langle dY | 1 \rangle = B dt^\alpha \]

(7)

We obtain from Eqs. (5,6) the generalized Fokker-Planck equation:

\[ dt_1 \partial_{t_1} \rho + dt_1^\beta \partial_{Y_1} (A \rho) = dt_1^\alpha \frac{1}{2} \partial_{Y_1}^2 (B \rho), \]

(8)

where \( \beta = \min(1, \alpha) \) is the leading exponent in \( dt \) of \( \langle dY | 1; 0 \rangle \), \( A(1; 0) = \langle dY / dt_1^\beta | 1; 0 \rangle \) plays the role of a generalized drift term and \( \rho = \rho(1|0) \).

The presence of time differentials of different order in Eq. (8) indicates that this equation is degenerate unless \( \alpha = 1 \), in which case also \( \beta = 1 \). In the subdiffusive case, we have \( \beta = \alpha < 1 \) and the PDF dynamics is governed by a balance between the drift and the diffusion, while the kinetic term \( dt_1 \partial_{t_1} \rho \) disappears. In the superdiffusive case \( \beta = 1 < \alpha \) and the diffusion term disappears. In this case Eq. (8) becomes a Liouville equation for the deterministic version of Eq. (3): \( dY / dt_1 = A(1; 0) \) and the probabilistic content of the problem is transferred to the initial distribution for \( Y_1 \) at \( t_1 \rightarrow t_0 \). The Markov case \( A(1; 0) = -BY_1 / 2 \) is recovered when \( C(t) = \exp(-B|t|/2) \). The fundamental solution \( \rho(1|0) \propto \exp\{-|Y_1 - Y_0|^2/(2Bt^\alpha)\} \) is obtained for \( t \ll B^{-1/\alpha} \) in the three ranges \( \alpha \gtrless 1 \) and \( \alpha = 1 \).

It is possible to complete the Kolmogorov pair associated with the stochastic process \( Y \), deriving a differential equation for the conditioning variable \( 0 \) in \( \rho(2|0) \). We consider the simpler case in which \( \alpha = 1 \) (notice that this does not imply that the process is Markovian). Setting \( t_0 = t_1 - \Delta t, \ t_1 < t_2 \), the backward equation can be obtained combining the
relation $\rho(2|0) = \int dY_1 \rho(2|1; 0) \rho(1|0)$ with $\rho(2|1; 0) = \rho(2; 0|1)/\rho(0|1)$ and $\rho(2; 0|1) = \rho(0|1; 2)\rho(2|1)$. The result is:

$$\rho(2|0) = \int dY_1 \rho(2|1) \rho_B(1|0; 2)$$

where

$$\rho_B(1|0; 2) = \rho(0|1; 2)\frac{\rho(1|0)}{\rho(0|1)}$$

Notice that in the Markov case, $\rho_B(1|0; 2) = \rho(1|0)$ and Eq. (9) takes the standard form $\rho(2|0) = \int dY_1 \rho(2|1) \rho(1|0)$. Invoking continuity, we can approximate the statistics for $\Delta Y$ as Gaussian at small time separations; indicating $t_0 = t_1 - dt$ and $t_2 = t_1 + dt$, we can then write:

$$\begin{cases}
\rho(0|1; 2) = c \exp\{-\frac{1}{2} (dW^2|1; 2)^{-1} |dY - \langle dY|1; 2 \rangle|^2\} \\
\rho(0|1) = c' \exp\{-\frac{1}{2} (dW^2|1)^{-1} |dY - \langle dY|1 \rangle|^2\} \\
\rho(1|0) = c'' \exp\{-\frac{1}{2} (dW^2|0)^{-1} |dY + \langle dY|0 \rangle|^2\}
\end{cases}$$

where $dY = Y_0 - Y_1$. Explicit expressions for $\rho_B$ can then be obtained substituting into Eq. (10). In the Gaussian case described by Eqn. (5) we would obtain:

$$\rho_B(1|0; 2) = c \exp\{-|dY - \tilde{A}dt|^2/(2Bdt)\}$$

where $c = e^{\gamma^2/2}$. Substituting Eq. (12) into (9) and Taylor expanding $\rho(2|1)$ around $Y_1 = Y_0$, a generalized backward Kolmogorov equation could then be written in explicit form ($dt_1 = -dt$):

$$[\partial_{t_1} - \tilde{A}\partial_{Y_1} + \frac{1}{2}B\partial_{Y_1}^2 + \tilde{S}]\rho(2|1) = 0$$

where $\tilde{S} = -[\partial_{Y_1} + 2A_M/B](A - A_M)$. In the Markov case, the standard form of the backward Kolmogorov equation is recovered: $A$ coincides with its Markovianized counterpart $A_M$, the source term $\tilde{S}$ vanishes and $\tilde{A} = -A$.

An application to ratchets

A simple application of the techniques illustrated so far is the determination of the equilibrium statistical properties of a ratchet field, via the generalized Fokker-Planck equation.
Specifically, consider the uniform one-dimensional Gaussian velocity field with correlation $C(x, t) = \langle u(0, 0) u(x, t) \rangle$:

$$C(x, t) = \exp\{-\frac{1}{2} [t^2 + 2\Lambda xt + x^2]\}, \quad |\Lambda| < 1$$

(14)

This velocity field has zero mean both in space and time, nonetheless it leads to a non-zero mean flow; in other words, it is a ratchet [10]. The drift and noise amplitude experienced by a particle in the velocity field $u(x, t)$ is obtained following the same procedure leading from Eqs. (4) to (5,6), just neglecting the initial condition at $t_0$ and defining $C_{ij} = \langle u(x(t_i), t_i) u(x(t_j), t_j) \rangle$. The result has a form analogous to Eq. (7):

$$\langle dW^2 | u \rangle = -2u^{-1} \langle du | u \rangle = [1 + 2\Lambda u + u^2] dt^2$$

(15)

thus, the stochastic process $u(t)$ is ballistic at short time scales. The equilibrium PDF of a particle travelling with velocity $u(x(t), t)$ will obey the generalized Fokker-Planck equation

$$\partial_u (\langle du | u \rangle \rho) = \frac{1}{2} \partial^2_u (\langle dW^2 | u \rangle \rho)$$

(16)

whose solution, from Eq. (15) is:

$$\rho(u) = c[1 + 2\Lambda u + u^2]^{-1} \exp(-u^2/2)$$

The ratchet mean flow will be given by the first moment of this distribution, plotted in Fig. 1.

An application to anomalous diffusion

As a second application, we determine the correlation between velocity and coordinate in a time and space homogeneous, unbiased, but otherwise generic diffusion process. In this case, $Y(t_1)$ indicates the coordinate of the walker with $Y(t_0) \equiv Y(0) = 0$, and $\rho(1|0)$ is the distribution of the walkers at time $t_1$. We have also:

$$\langle |Y(t_2) - Y(t_1)|^2 \rangle = \langle B(1; 0)|1\rangle \Delta t^\alpha = B(1) \Delta t^\alpha$$

(17)

with $B(1) = B$ constant from homogeneity of the process. The velocity averaged at scale $\Delta t$ is $\Delta Y/\Delta t$; using the definition $A(1; 0) = \langle dY/dt^\beta |1; 0\rangle$, with $\beta = \min(1, \alpha)$ [see Eq. (5)], we have:

$$\langle Y \Delta Y/\Delta t \rangle = \Delta t^{(\beta-1)} \langle YA \rangle$$

(18)
We have seen that, in the three regimes $\alpha \gtrsim 1$ and $\alpha = 1$, the generalized Fokker-Planck equation (8) takes the form:

$$\begin{align*}
\partial_t \rho(t_1) + \partial_{Y_1} \left[ A(1; 0) \rho(1|0) \right] &= 0, \quad \alpha > 1 \\
\partial_t \rho(1|0) + \partial_{Y_1} \left[ A(1; 0) \rho(1|0) \right] &= \frac{1}{2} \partial_{Y_1}^2 \left[ B(1; 0) \rho(1|0) \right], \quad \alpha = 1 \\
A(1; 0) \rho(1|0) &= \frac{1}{2} \partial_{Y_1} \left[ B(1; 0) \rho(1|0) \right], \quad \alpha < 1
\end{align*}$$

Multiplying these equations by appropriate powers of $Y(t_1)$ and taking averages, we obtain, using Eqs. (17,18):

$$2 \langle Y \Delta Y / \Delta t \rangle = \begin{cases} 
\alpha B t^{\alpha - 1}, & \alpha > 1 \\
0, & \alpha = 1 \\
- B \Delta t^{\alpha - 1}, & \alpha < 1
\end{cases} \quad (19)$$

which gives a quantitative content to the concepts of persistence and antipersistence in generic diffusion processes.

Further applications of the present Fokker-Planck approach are limited by the fact that several operations, natural for Markovian processes, become tricky in the general case. The central issue appears to be the multiplicity of drift and diffusion coefficients generated by different conditioning choices.

This has the important consequence that the only physical solutions of equations like (8) are those at statistical equilibrium. For instance, if we considered the version of Eq. (8)
obtained from the unconstrained moments of Eq. (7), we would obtain an evolution equation for the one-time PDF \( \rho_0(Y) \), which could be solved for an arbitrary, out of equilibrium initial condition \( \tilde{\rho}_0(Y) \). This, however, would produce a Markovianized time dependent statistics losing all the scaling properties of the original process. The right evolution is given by:

\[
\tilde{\rho}(1) = \int dY_0 \rho(1|0) \tilde{\rho}_0(Y_0)
\]

In other words, conditioning is necessary to determine the evolution of an out of equilibrium one-time PDF. On the same line of reasoning, we find that the evolution described by Eqs. (5,6,8) (that is conditioned only at one time) is unable to account for the aging of the process, which may be defined, including the possibility of non-renewing processes, as the approach to equilibrium of the correlation \( \langle Y(t_2)Y(t_1)|0 \rangle \) as \( t_0 \to -\infty \). In this case, taking \( t_2 > t_1 \),

\[
\langle Y(t_2)Y(t_1)|0 \rangle = \langle \langle Y(t_2)|1;0 \rangle Y(t_1)|0 \rangle
\]

would require evaluation of \( \langle Y(t_2)|1;0 \rangle \) by means of a version of the generalized Fokker-Planck equation (8) conditioned at two times.

Thus, in general, to determine non-equilibrium statistics conditioned at \( n \) times, it is necessary to consider a generalized Fokker-Planck equation with moments conditioned at \( n + 1 \) times.

These problems limit also the applicability of a Monte Carlo approach based on the fictitious trajectories defined in Eq. (3). Consider for instance the motion of a particle moving with velocity \( Y \). One may try to obtain the displacement statistics by Monte Carlo integration of the generalized Langevin equation (3), coupled with the kinematic condition on the particle coordinate \( x(t) \): \( dx = Y dt \). The first moment of the displacement is evaluated correctly:

\[
\langle x(t)|0 \rangle = x(0) + \int_0^t d\tau_1 \langle Y(t_1)|0 \rangle
\]

and \( \langle Y(t_1)|0 \rangle \) is generated averaging over the trajectories determined by Eq. (3). But, suppose we wish to calculate the second moment; we have:

\[
\langle [x(t) - x(0)]^2 \rangle = 2 \int_0^t d\tau_1 \int_{\tau_1}^{t} d\tau_2 \langle Y(t_1)Y(t_2) \rangle
\]

with

\[
\langle Y(t_2)Y(t_1) \rangle = \langle \langle Y(t_2)|1;0 \rangle Y(t_1) \rangle.
\]
The situation is analogous to Eq. (20) and the conditional average $\langle Y(t_2)|1;0 \rangle$ is evaluated correctly by a Monte Carlo with conditioning at a single time, only in the Markov case, when $\langle Y(t_2)|1;0 \rangle = \langle Y(t_2)|1 \rangle$.

What happens is that $x(t)$ depends on the whole history of $Y$. To obtain the full $x(t)$ statistics, the conditional moments entering Eq. (3) should be substituted at time $\tau < t$ by others depending not only on $Y(\tau)$ and $Y(0)$, but also on $x(\tau)$, which is equivalent to adopting a non-local approach like the one in [6]. (Hence, the result in [8] on the Lagrangian correlation time in a uniform Gaussian velocity field, which neglects this conditioning, has at most value of estimate).

Another set of questions relate to the existence of a stochastic process, for a given choice of drift and diffusion coefficients, and, conversely, to the uniqueness of the generalized Fokker-Planck equation associated to a given process.

As regards the first question, at least if we want to construct a stationary process, it turns out that the choice of drift and diffusion coefficient in Eq. (7) is not free, and the functions $A(1;0), B(1;0)$ have to be chosen together with the one- and two-time PDF’s $\rho(1)$ and $\rho(1|0)$: it is not enough to impose that $A$ and $B$ depend solely on time differences.

In fact, from $A(1;0)$ and $B(1;0)$, if the process were stationary, it would be possible, taking the limit $t_1−t_0 \to \infty$ in $A(1;0)$ and $B(1;0)$, to calculate the unconditioned moments $A(1)$ and $B(1)$, and, using the unconditioned version of Eq. (8), the one-time equilibrium PDF $\rho(1)$. At the same time, knowing $A(1)$ and $B(1)$ would give the form of the transition PDF $\rho(1|0)$ for $t_1−t_0 \to 0$, to be used as initial condition for Eq. (8) in the calculation of $\rho(1|0)$ at finite time separations. Under these conditions, $\rho(1)$ and $\rho(1|0)$ would be determined by the pair $\{A(1;0), B(1;0)\}$ in the two regimes in which $t_1−t_0$ is infinite and finite, respectively. It would then be easy to construct profiles of $A(1;0)$ and $B(1;0)$, fixed $A(1)$ and $B(1)$, such that the condition $\rho(1) = \int \rho(1|0)\rho(0)dY_0$ be not satisfied for finite $t_1−t_0$, which is absurd.

In conclusion, contrary to the Markov case, to be able to write down a generalized Fokker-Planck equation, it would be necessary to know in advance the form of the transition PDF that is its solution; a characteristic shared by the approach in [12]. The main content of an equation like (8) seems therefore just to establish a relation, which should be satisfied by any experimentally measured stochastic time series, between the transition PDF $\rho(1|0)$
and the conditional moments $\langle dY|1;0 \rangle$ and $\langle dY^2|1;0 \rangle$.

Turning to the uniqueness issue, we observe that the generalized Fokker-Planck equation (8), given a transition PDF $\rho(1|0)$, does not fix by itself the form of the drift and diffusion coefficients $A(1;0)$ and $B(1;0)$. In order for that equation to have a probabilistic content, it is necessary that the consistency condition

$$\langle g|1 \rangle = \int dY_0 \langle g|1;0 \rangle \rho(0|1) = \int dY_0 \langle g|1;0 \rangle \frac{\rho(1|0)\rho(0)}{\rho(1)}$$

(22)

be satisfied for $g = \Delta Y, \Delta W^2$. However, this condition, together with Eq. (8) is still not sufficient to fix $A(1;0)$ and $B(1;0)$.

To prove this, the following simple example is sufficient. Consider a space and time homogeneous, unbiased diffusion process. Again, $Y$ indicates the walker coordinate. From space homogeneity, $\langle \Delta W^2|1;0 \rangle$ and $\rho(0|1)$ must be function only of $Y(t_1) - Y(t_0)$ and, from the process being unbiased, both functions must be even. Again from the process being unbiased, $\langle \Delta Y|1;0 \rangle$ must be an odd function of $Y(t_1) - Y(t_0)$ and $\langle \Delta Y|1 \rangle$ must be identically zero. We see then that the definition

$$\int dY_0 \langle \Delta W^2|1;0 \rangle \rho(0|1) = \langle \Delta W^2|1 \rangle = B\Delta t^\alpha$$

is satisfied by the general solution

$$\langle \Delta W^2|1;0 \rangle = B\{1 + c[1 - \frac{g(1;0)}{\langle g|1 \rangle}])\} \Delta t^\alpha$$

where $g(1;0) = g(Y_1 - Y_0, t_1 - t_0)$ is generic and $c$ is chosen so that $\langle \Delta W^2|1;0 \rangle$ remains positive defined. Substituting into the generalized Fokker-Planck equation (8), and solving for $A(1;0)$, we see that the result is an odd function of $Y(t_1) - Y(t_0)$, so that $A(1) = \langle A(1;0)|1 \rangle$ remains zero independently of $g$.

Thus, uniqueness is not guaranteed in general. However, in order for Eq. (22) to be satisfied, it is still necessary that the moments of $\rho(2|1;0)$ and $\rho(2|1)$ be of the same order in $\Delta t$. This property is not satisfied by the Fokker-Planck equation derived in [12], assuming that, irrespective of $\alpha$, $\langle dY|1;0 \rangle$ and $\langle dW^2|1;0 \rangle$ be both $O(\Delta t)$. Like the approach in this letter, also the one in [12] can be seen as a reconstruction technique of the transition PDF $\rho(1|0)$, based on the use of fictitious trajectories. In the case of [12], however, not only have the trajectories a memory of the past limited to the discrete time $t_0$, but, imposing
the local Poisson-like behavior $dY \sim dt^{1/2}$, they loose also all information on the local structure of the real trajectories. This clearly precludes any application of the type leading to Eq. (19).

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