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Singular Boundaries in the Forward Chapman-Kolmogorov Differential Equation

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Abstract The forward Chapman-Kolmogorov differential equation is used to model the time evolution of the Probability Density Function of fluctuations. This equation may be restricted to either Master, Fokker-Planck or Liouville equations. A derivation of the Liouville equation with possible singular boundary conditions has already been presented in a previous publication (Valiño and Hierro in Phys. Rev. E 67:046310, 2003). In this paper, that derivation is extended to the full Chapman-Kolmogorov differential equation.

Keywords Probability density function · Singular boundaries

1 Introduction

The derivation of the Chapman-Kolmogorov differential equation as a model to represent the evolution of a Probability Density Function (PDF) may be found in [9]. In Fluid Dynamics, for instance, PDF methods are extensively used to model turbulent fluctuations [3, 4, 19]. Fokker-Planck equations, statistically equivalent to the original Navier-Stokes equations, are derived by different means: either from the closed, multipoint Hopf functional, or from the definition of the PDF as the expected value of a Dirac's delta, or from a weak formulation where the PDF is considered as a functional acting on a space of test functions. Recently [16], there has been presented a derivation of the Fokker-Planck equations, with boundary conditions included, from the full Chapman-Kolmogorov differential equations [9] oriented towards problems with fast surface transport. That methodology [16] closely resembles, in the initial steps, the one followed in this paper, although significant overall differences are apparent.

In a typical derivation, there are some surface integrals which could lead to singularities at the boundaries of the phase space domain which are neglected based either on “a priori” assumptions on the properties of the test functions, or on “a posteriori” boundary conditions imposed on the problem from physical considerations. However, there are some situations

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where the presence of a singularity or a discontinuity at the boundary of the probabilistic space can have a physical meaning. Kuznetsov and Sabelnikov [15] proved that, in the PDF of scalar concentration fields with external intermittence, the contribution of the laminar zones creates a singularity at the boundary of the probability space. This problem was also studied by Klimenko and Bilger [13]. Not only that, one can also think of situations where the global probability is not preserved; for instance, a compressible flow inside a fixed volume connected to an external reservoir of fluid. In that example, there is an additional term in the Fokker-Planck equation which is linear in the PDF itself and may be modelled by a global renormalization of the weight of Monte Carlo particles after each time step [21]. Lubashevsky et al. [16] analysed a situation where there may be present a discontinuity on the transport properties at the boundary, a fast diffusion layer, and computed the value of the corresponding additional surface terms from physical models for the stochastic behaviour close to the boundary.

In a previous publication [21], Liouville equations with possible singular boundary conditions were analysed. In this paper, the full Chapman-Kolmogorov differential equation with possible singular boundary conditions is studied following Gardiner's weak derivation [9]. All the surface terms are retained and analysed in this paper, in the most general formulation of those found in the literature. The only restriction posed on test functions is for them to be twice continuously differentiable, class C^2, and integrable with a measure given by the probability whose evolution is computed. The inclusion of a diffusion term means that the drift term stops being a proper first-order tensor, as it happens in the Liouville equation, and some care must be taken to rearrange different non-tensorial quantities so that proper tensors may be handled as required by a systematic application of Reynolds' transport and divergence theorems.

2 Definition of the PDF

Work is done in a stochastic phase space made of an M dimensional open region $G \in \mathbb{R}^M$, an M manifold, plus a piecewise smooth boundary S, an $M-1$ manifold. $G_1 = \mathbb{R}^M \backslash \overline{G}$ will be considered as an external reservoir if there is some inflow or outflow of probability from $\overline{G}$. There are possible singular contributions to the PDF on the surface S. The normal to S, pointing from G to G_1, will be referred to as $\boldsymbol{n}$. Were there inner singularities, it would always be possible to split the inner domain so that the singularities were located at the new boundaries and compute explicitly the exchanges of probability between the new domains. It will also be assumed that the PDF may be normalized to a global weight unity; this means that singularities at the boundary may be simple layers [22], but multilayers are excluded. Inside G, the PDF is of class C^2. Einstein's summation convention on repeated (mute) indices is followed except when placed within parentheses.

The full (inner plus boundary) PDF may be written as

$$P(z;t) = P^+(z;t) + \gamma_S(z,t)\delta_S \tag{1}$$

where P^+ stands for the inner contribution, δ_S is the simple layer functional defined on S and γ_S is a local weight associated to each boundary point, t is time, z is used to represent the different components of the phase space. The lack of a singular contribution in some or all the points of the boundary may be represented by a zero value of γ_S at them. The semicolon symbol between z and t is used to denote that z correspond to variables of the stochastic phase space whereas t does not. Normalization means, by using the properties of a simple layer functional [22], that

$$\int_G P^+(z;t)\,d^M z + \oint_S \gamma_S(z,t)\,dS = 1 \tag{2}$$

where $d^M z$ is a short-hand notation for the differential form $dz^1 \wedge dz^2 \wedge \cdots \wedge dz^M$, dS is a surface element of the boundary surface with a local surface metrics, $a_{\alpha\beta}$, defined by the restriction of the global metrics, g_{ij}, used in $\mathbb{R}^M$ to the $M-1$ manifold S, $dS = \sqrt{|\det a_{\alpha\beta}|}d\zeta^1 \wedge d\zeta^2 \wedge \cdots \wedge d\zeta^{M-1} = a^{1/2}d^{M-1}\zeta$, with $\boldsymbol{\zeta}$ representing the $M-1$ coordinates of the $M-1$ manifold S, Greek indices are used to represent coordinates restricted to S. A volume element in either G or G_1 is $dV = \sqrt{|\det g_{ij}|}dz^1 \wedge dz^2 \wedge \cdots \wedge dz^M = g^{1/2}d^M z$. Usually, the stochastic phase space is Euclidean with a Cartesian basis, namely $g^{1/2} = \sqrt{|\det g_{ij}|} = 1$ and $dV = dz^M$; however, the use of generalised coordinates will be preserved during the derivation. It should be noticed that P^+ do not transform as a scalar field under a coordinate change [20]. By definition, $P^+ d^M z = P'^+ d^M z'$ under a change of coordinates from z to z'; therefore, $P'^+ = P^+ J$, where J is the Jacobian of z as a function of z'. It is also a well-known fact [1] that $g'^{1/2} = g^{1/2}J$. It is immediate to check that the volume weight $\overline{P^+} = P^+ g^{-1/2}$ is a scalar field and that, with an Euclidean metrics, scalar weights coincide with PDF's. On the other hand, γ_S is not a surface PDF, but the scalar weight of a simple layer functional; $P_S = \gamma_S\sqrt{|\det a_{\alpha\beta}|} = \gamma_S a^{1/2}$ is the surface PDF related to the γ_S scalar weight. Equation (2) can be rewritten as

$$\int_G \overline{P^+}(z;t)\,dV + \oint_S \gamma_S(z,t)\,dS = \int_G P^+(z;t)\,d^M z + \oint_S P_S(z,t)\,d^{M-1}\zeta = 1 \tag{3}$$

with a consistent grouping of volume and surface PDF's on one side and of volume and surface scalar weights on the other one.

3 Evolution of the PDF with Singularities at the Boundaries

Equation (3.4.16) of [9] may be used as a starting point for the derivation of the time evolution of P. Moreover, an integration over $\boldsymbol{y}$ may be carried out with the only consequence that probabilities at time t conditional on probabilities at time t' are transformed into probabilities at time t regardless of their origin. Formulae are shorter after this integration, whereas derivations are not modified since there are no operators acting on the previous time variables. Using the naming conventions of this paper and studying probabilities regardless of their origin, this starting point becomes

$$\begin{aligned}
&\frac{d}{dt}\Big[\int f(z)P(z;t)\,d^M z\Big] \\
&\quad = \int \Big[A^i(z,t)\frac{\partial f(z)}{\partial z^i} + \frac{1}{2}B^{ij}(z,t)\frac{\partial^2 f(z)}{\partial z^i \partial z^j}\Big]P(z;t)\,d^M z \\
&\qquad + \int f(z)\Big\{⨍\big[W(z|\boldsymbol{x};t)P(\boldsymbol{x};t) - W(\boldsymbol{x}|z;t)P(z;t)\big]d^M x\Big\}\,d^M z
\end{aligned} \tag{4}$$

where $f(z)$ represents a generic test function in the phase space which is twice continuously differentiable, the symbol $⨍$ is used to denote a principal value integral where a small neighbourhood $|\boldsymbol{x} - z| < \varepsilon$ is excluded. By comparison of (3.4.15) and (3.4.16) of [9], an obvious typo has been corrected. In the original reference, partial time derivatives are used instead of total time derivatives; this difference is only relevant if the phase space reference system is time-dependent. $W(\boldsymbol{x}|z;t)$, $A^i(z,t)$ and $B^{ij}(z,t)$ stand for [9]

$$W(\boldsymbol{x}|z;t) = \lim_{\Delta t\to 0} P(\boldsymbol{x};t+\Delta t|z;t)/\Delta t \quad \text{for } |\boldsymbol{x}-\boldsymbol{z}| \geq \varepsilon \tag{5}$$

$$A^i(z,t) = \lim_{\Delta t\to 0} \frac{1}{\Delta t} \int_{|\boldsymbol{x}-z|<\varepsilon} (x^i - z^i) P(\boldsymbol{x};t+\Delta t|\boldsymbol{z};t) d^M x + O(\varepsilon) \tag{6}$$

$$B^{ij}(z,t) = \lim_{\Delta t\to 0} \frac{1}{\Delta t} \int_{|\boldsymbol{x}-z|<\varepsilon} (x^i - z^i)(x^j - z^j) P(\boldsymbol{x};t+\Delta t|\boldsymbol{z};t) d^M x + O(\varepsilon) \tag{7}$$

W is the jump term, it represents a discontinuous evolution at discrete points in the path of a Monte Carlo particle; A^i is the drift term, it represents a continuous, differentiable path; and B^{ij} is the diffusion term, it represents a continuous, non-differentiable path. All higher order terms (higher order in $\boldsymbol{x}-\boldsymbol{z}$) vanish when $\varepsilon \to 0$.

It must be remembered throughout the paper that $P^+ d^M z = \overline{P^+} dV$ and $P_S d^{M-1}\zeta = \gamma_S dS$.

3.1 Inertial Term

The term on the left hand side (4) is referred to, from now on, as inertial by analogy with similar terms in mechanics and is the first one to be expanded. The existence of moving boundaries [5], with velocity in phase space $\dot{\boldsymbol{z}}_S$ is not excluded. For instance, in the stochastic analysis of pure diffusion problems, fluctuations tend to zero, shrinking G and moving S in the process. This means that the difference between partial and total time derivatives should be taken into account since there is a distinction between a coordinate system which remains fixed at time t and a coordinate system moving with the same velocity as S at the boundary.

$$\begin{aligned}
&\frac{d}{dt}\int f(z) P(z;t)\, d^M z \\
&\quad \overset{1}{=} \frac{d}{dt}\Big[\int f(z)\overline{P^+}(z;t)\, dV + \oint f(z)\gamma_S(z,t)\, dS\Big] \\
&\quad \overset{2}{=} \int f \frac{\partial \overline{P^+}}{\partial t} dV + \oint f\overline{P^+}\dot{z}^i_S n_i\, dS + \oint \Big[\frac{df\gamma_S}{dt} + f\gamma_S \frac{1}{2a}\frac{\partial a}{\partial t} + f\gamma_S \dot{\zeta}^\alpha_{;\alpha}\Big] dS
\end{aligned} \tag{8}$$

where scalar weights have been used in equality 1 because in equality 2 the Reynolds transport theorem for volumes and surfaces [1] is applied and this theorem requires tensorial integrands. $\dot{\boldsymbol{z}}_S$ represents the velocity field that $\overline{G}$ is moving with, its divergence is the time derivative of the natural logarithm of the ratio of the volume element at a given time to its initial value, $dV = J dV_0$, $\dot{z}^i_{S;i} = d\ln J/dt$. $\dot{\boldsymbol{z}}_S$ at S is the propagation velocity of the moving boundary S. $\dot{\zeta}^\alpha_{;\alpha} = \dot{z}^\alpha_{S;\alpha}$ is its divergence restricted to the boundary S. It can be computed, as if there were no component normal to S, in coordinates intrinsic to S, $\boldsymbol{\zeta}$. $\dot{a} = da/dt = \partial a/\partial t$ has been assumed [1] since intrinsic coordinates $\boldsymbol{\zeta}$ are chosen so that S propagates with a velocity normal to itself when viewed from the outside $\mathbb{R}^M$ space.

When writing $dV = J dV_0$ some care must be taken with the definition of coordinates. In principle, one may work with a fixed coordinate system which covers $\mathbb{R}^M$ and whose metrics is the intrinsic metrics of $\mathbb{R}^M$ which is assumed to remain fixed in time; if the integration volume is moving, this shows as volume integral with time-dependent limits. On the other hand, one could also work in a coordinate system moving with the same velocity as the integration volume, such that the coordinates of a point remain the same as those of the initial time and the metrics is modified to take into account the possible presence of dilatation or contraction; the integration limits of a volume integral are now fixed (thus, time derivatives may come inside the integral), but the metrics linked to a volume element is modified. It is in this second class of coordinate systems where expressions like $dV = J dV_0$ make sense. Of course, after performing the formal calculations in a moving coordinate system, the fixed coordinate system may be recovered as it is the standard practice in the derivation of Reynolds' transport theorem.

In the last integral of (8), $df\gamma_S/dt$ requires some care. A generic f has no explicit dependence on time; however, it depends on both the surface coordinates and the coordinate normal to S, since it is a volume scalar; on the other hand, γ_S and a show an explicit dependence on time but, in the phase space, they only depend on surface coordinates, they are surface scalar fields. Thus,

$$\begin{aligned}\frac{df\gamma_S}{dt} + f\gamma_S\dot{\zeta}^\alpha_{;\alpha} + \frac{f\gamma_S}{2a}\dot{a} &= f\frac{\partial\gamma_S}{\partial t} + \frac{\partial f\gamma_S}{\partial\zeta^\alpha}\dot{\zeta}^\alpha + \gamma_S\frac{\partial f}{\partial z_S^{(n)}}\dot{z_S}^{(n)} + f\gamma_S\dot{\zeta}^\alpha_{;\alpha} + \frac{f\gamma_S}{a^{1/2}}\frac{\partial a^{1/2}}{\partial t}\\ &= f\frac{\partial\gamma_S}{\partial t} + \frac{f\gamma_S}{a^{1/2}}\frac{\partial a^{1/2}}{\partial t} + \gamma_S\frac{\partial f}{\partial z_S^{(n)}}\dot{z_S}^{(n)} + (f\gamma_S\dot{\zeta}^\alpha)_{;\alpha} \qquad (9)\end{aligned}$$

where $\dot{z}_S^n$ and $\partial/\partial z_S^n$ are short-hand notations for $\dot{z}_S^i n_i$ (the propagation velocity of the surface normal to itself) and $n_j\partial/\partial z_S^j$ (gradient in a direction normal to the surface), respectively. If (9) is replaced into (8), the divergence theorem may be applied to the last term of (9) which is transformed into a flow through the boundary of S; however, S is, in its turn, a boundary and the boundary of a boundary is the empty set [18], therefore, this contribution is zero. On the other hand surface integrals can be converted into volume integrals, provided that the integrand is multiplied by the appropriate layer functional. If the integrand of the surface integral has no normal derivatives, the simple layer functional defined on S is only needed; if there is a normal derivative, the double layer functional must be used [22]

$$\oint \gamma_S\dot{z}_S^{(n)}\frac{\partial f}{\partial z_S^{(n)}}\,dS = -\int f\frac{\partial(\gamma_S\dot{z}_S^{(n)}\delta_S)}{\partial z_S^{(n)}}\,dV$$

Using layer functionals and neglecting zero terms, (8) becomes

$$\begin{aligned}\frac{d}{dt}\int f(z)P(z;t)\,d^Mz = \int f\Big[\frac{\partial\overline{P^+}}{\partial t} + \Big(\frac{\partial\gamma_S}{\partial t} + \frac{\gamma_S}{a^{1/2}}\frac{\partial a^{1/2}}{\partial t} + \overline{P^+}\dot{z}_S^n\Big)\delta_S\\ - \frac{\partial(\gamma_S\dot{z}_S^{(n)}\delta_S)}{\partial z_S^{(n)}}\Big]\,dV \qquad (10)\end{aligned}$$

If the boundary S were not included in the region where the PDF is defined, (8) would retain only the volume integral in the first equality and (10) would be replaced by

$$\frac{d}{dt}\int f(z)P(z;t)\,d^Mz = \int f\Big[\frac{\partial\overline{P^+}}{\partial t} + \overline{P^+}\dot{z}_S^n\delta_S\Big]\,dV \qquad (11)$$

The full space comprises $\overline{G}\cup G_1$ and it is not excluded the possibility of probability exchanges between $\overline{G}$ and G_1. Since S is included in $\overline{G}$ but excluded from G_1, (10) represents the inertial term in $\overline{G}$ and (11) in G_1. Both inertial terms contain a contribution proportional to δ_S; that is to say, both may contribute to the appearance of a simple layer singularity at S. In G_1 the contribution to the singularity has a weight $\overline{P^+_{G1}}\dot{z}^i_S n_i$ with $\boldsymbol{n}$ pointing from G_1 to G and $\overline{P^+_{G1}}$ being the limit of $\overline{P^+}$ as S is approached from G_1; on the other hand, in G there is a contribution $\overline{P^+_G}\dot{z}^i_S n_i$ with $\boldsymbol{n}$ pointing from G to G_1 and $\overline{P^+_G}$ being the limit of $\overline{P^+}$ as S is approached from G. It means that, if there is some inertial probability flow from G_1 to S, the inertial variation of the simple layer at S will be given by

$$\int f\Big(\frac{\partial \gamma_S}{\partial t}+\frac{\gamma_S}{a^{1/2}}\frac{\partial a^{1/2}}{\partial t}-\big[\overline{P^+}\big]^S\dot{z}^n_S\Big)\delta_S\,dV \tag{12}$$

where $[\overline{P^+}]^S=(\overline{P^+_{G1}}-\overline{P^+_G})|_S$ and $\boldsymbol{n}$ points from G to G_1. Remember that test functions are C^2 in $\mathbb{R}^M$ and, thus, they do not have discontinuities in S. The full inertial contribution to the evolution of scalar weights is given by

$$\int f\Big[\frac{\partial \overline{P^+}}{\partial t}+\Big(\frac{\partial \gamma_S}{\partial t}+\frac{\gamma_S}{a^{1/2}}\frac{\partial a^{1/2}}{\partial t}-\big[\overline{P^+}\big]^S\dot{z}^n_S\Big)\delta_S-\frac{\partial(\gamma_S\dot{z}^{(n)}_S\delta_S)}{\partial z^{(n)}_S}\Big]dV \tag{13}$$

Equation (13) may be rearranged to provide the full inertial contribution to the evolution of the PDF, recalling that $\overline{P^+}g^{1/2}=P^+$, $\gamma_S a^{1/2}=P_S$, and $g^{1/2}$ has no time dependence in the fixed coordinate system,

$$\int f\frac{\partial P^+}{\partial t}d^Mz+\oint f\Big(\frac{\partial P_S}{\partial t}-\big[P^+\big]^S\frac{a^{1/2}}{g^{1/2}}\dot{z}^n_S\Big)d^{M-1}\zeta+\oint\frac{\partial f}{\partial z^{(n)}_S}\dot{z}^{(n)}_S P_S\,d^{M-1}\zeta \tag{14}$$

3.2 Drift and Diffusion Terms

Drift and diffusion terms, the first and second contribution on the right hand side of (4) are analysed together. The reason is that neither A^i, nor $\partial^2 f/\partial z_i\partial z_j$ are tensorial quantities, though they may be rearranged in a tensorial way when jointly studied. The evolution due to drift and diffusion terms may be related to a Stochastic Differential Equation (SDE) [9, 20] in variable $\boldsymbol{z}$ solved by means of a Monte Carlo method where the particles follow continuous, non-differentiable paths; jumps may be added as a discrete set of discontinuities in the corresponding paths. The SDE, see (15), may be understood either in the Ito sense [9] or in the Stratonovich sense [20].

$$dz^i=h^i dt+g^{ia}dW_a \tag{15}$$

where dW_a represents the time differential of an M-dimensional set of Wiener processes which are not affected by a change of variables, $\boldsymbol{W}$ represents a set of scalars with labels instead of a covector as could be expected.

In the Stratonovich interpretation [20], h^i and g^{ia} are contravariant vectors (with an additional set of labels in the second case); however, drift and diffusion coefficients, as given by (6) and (7), are $A^i=h^i+(1/2)g^{ka}\partial g^{ia}/\partial z^k$ and $B^{ij}=g^{ia}g^{ja}$. This translates into the following transformation laws for drift and diffusion coefficients, where a generic time-dependent change of variables from $\boldsymbol{z}$ to $\boldsymbol{z}'$ has been assumed,

$$A'^i=\frac{\partial z'^i}{\partial t}+\frac{\partial z'^i}{\partial z^k}A^k+\frac{1}{2}\frac{\partial^2 z'^i}{\partial z^m\partial z^n}B^{mn} \tag{16}$$

$$B'^{ij} = \frac{\partial z'^i}{\partial z^m} \frac{\partial z'^j}{\partial z^n} B^{mn} \tag{17}$$

It should be noticed that in the original reference [20], the $1/2$ factor in the last term of (16) is absent. The reason is that the time differential of the Wiener process, the Langevin force, is normalized so that $\langle dW_a(t)dW_b(t)\rangle = 2\delta_{ab}dt$, whereas in this article it is assumed that $\langle dW_a(t)dW_b(t)\rangle = \delta_{ab}dt$ as in [9].

In the Ito interpretation [9], drift and diffusion coefficients, as given by (6) and (7), come straightforwardly from the SDE, $A^i = h^i$ and $B^{ij} = g^{ia}g^{ja}$. However, $h^i = A^i$ stops obeying the rules of ordinary calculus under change of variables; not surprisingly, the application of the many variables Ito calculus leads to the same rules as (16) and (17) for the transformation of drift and diffusion coefficients. In the original formula to compare with, (4.3.17) of [9], an explicit time dependence of the change of variables is not considered; so, the $\partial z'^i/\partial t$ term of (16) is lacking there.

In any event, with either Stratonovich or Ito interpretations, the result is the same: the diffusion coefficient, B^{ij}, is a second-order contravariant tensor, but the drift coefficient, A^i, is not. The $\partial z'^i/\partial t$ contribution is a Galilean transformation of velocities and poses no problem; in the absence of diffusion [21], A^i behaves as a contravariant velocity vector defined in phase space where, if needed, a zero time coordinate with $A^0 = 1$, $B^{00} = B^{0i} = B^{i0} = 0$ and $t' = z'^0 = t = z^0$ could be added. The last term of (16) is the one which precludes proper tensorial behaviour when there is a non-zero diffusion coefficient.

Since f is a scalar, $\partial f/\partial z^j$ a covector, and $f_{;kl} = \partial^2 f/\partial z^k \partial z^l - \Gamma^i_{kl} f_{;i}$ a second order $(0,2)$ tensor (Γ^i_{kl} is the Christoffel symbol); the drift plus diffusion contributions to the integrand on the right of (4) may be rewritten as,

$$A^i \frac{\partial f}{\partial z^i} + \frac{B^{ij}}{2} \frac{\partial^2 f}{\partial z^i \partial z^j} = A^i f_{;i} + \frac{B^{kl}}{2}(f_{;kl} + \Gamma^i_{kl} f_{;i}) = \left(A^i + \frac{B^{kl}}{2}\Gamma^i_{kl}\right) f_{;i} + \frac{B^{kl}}{2} f_{;kl} \tag{18}$$

which should transform as a scalar as the inertial term does. $\overline{P}$ has been extracted as a common scalar factor. The last term on the right of (18) is already a scalar (the double contraction of a second-order contravariant tensor with a second-order covariant tensor) whereas the remaining term is $A^i + \Gamma^i_{kl}B^{kl}/2$ contracted with a covector, $f_{;i}$, so $A^i + \Gamma^i_{kl}B^{kl}/2$ should be a vector. This is checked next

$$\begin{aligned}
\frac{\partial z'^j}{\partial z^i}\left(A^i + \Gamma^i_{kl}\frac{B^{kl}}{2}\right) &\overset{1}{=} \frac{\partial z'^j}{\partial z^i} A^i + \frac{B'^{mn}}{2}\left[\frac{\partial z'^j}{\partial z^i}\Gamma^i_{kl}\frac{\partial z^k}{\partial z'^m}\frac{\partial z^l}{\partial z'^n} + \frac{\partial z'^j}{\partial z^i}\left(\frac{\partial^2 z^i}{\partial z'^m \partial z'^n} - \frac{\partial^2 z^i}{\partial z'^m \partial z'^n}\right)\right] \\
&\overset{2}{=} \frac{\partial z'^j}{\partial z^i} A^i + \frac{\partial^2 z'^j}{\partial z^p \partial z^q}\frac{\partial z^p}{\partial z'^m}\frac{\partial z^q}{\partial z'^n}\frac{B'^{mn}}{2} + \Gamma'^j_{mn}\frac{B'^{mn}}{2} \\
&\overset{3}{=} \frac{\partial z'^j}{\partial z^i} A^i + \frac{\partial^2 z'^j}{\partial z^p \partial z^q}\frac{B^{pq}}{2} + \Gamma'^j_{mn}\frac{B'^{mn}}{2} = A'^j + \Gamma'^j_{mn}\frac{B'^{mn}}{2}
\end{aligned} \tag{19}$$

In equality 1, the tensorial behaviour of B^{kl} has been used to express its old components as a function of the new ones, B'^{mn}, and an additional quantity has been added and subtracted. In equality 2, the transformation law of Christoffel symbols [1] is used whereas the remaining term is rewritten in a different way [6] with second derivatives of the new coordinates instead of second derivatives of the old coordinates. In equality 3, the diffusion tensor is expressed in the old components and the transformation law given by (16), after separation of the Galilean transformation, is finally applied.

An alternative rearrangement of A^i, B^{ij} and $\partial^2 f/\partial z^i \partial z^j$ has been proposed by Graham [10, 20]. He showed that $A^i - (1/2)g^{-1/2}\partial(g^{1/2}B^{ij})/\partial z^j$ transforms as a contravariant vector; it must be noticed that, in the original reference, a contravariant metrics is used instead of a covariant one, so the sign of the exponential of the determinant of the metrics is reversed, and the $1/2$ factor is lacking for the reason previously explained. However, both rearrangements may be easily proved to be related

$$B^{ik}_{;k} = \frac{\partial B^{ik}}{\partial z^k} + \Gamma^k_{lk}B^{il} + \Gamma^i_{kl}B^{kl} = g^{-1/2}\frac{\partial g^{1/2}B^{ik}}{\partial z^k} + \Gamma^i_{kl}B^{kl} \tag{20}$$

where it has been assumed that work is done with a connection compatible with the metrics, $-g^{-1/2}\partial(g^{1/2}B^{ij})/\partial z^j = \Gamma^i_{kl}B^{kl} - B^{ij}_{;j}$, where $B^{ij}_{;j}$ is a contravariant vector which can be added and subtracted to (18) to obtain

$$A^i\frac{\partial f}{\partial z^i} + \frac{1}{2}B^{ij}\frac{\partial^2 f}{\partial z^i \partial z^j} = \left(A^i - \frac{1}{2g^{1/2}}\frac{\partial g^{1/2}B^{ij}}{\partial z^j}\right)f_{;i} + \frac{1}{2}(B^{ij}f_{;i})_{;j} \tag{21}$$

where the last term on the right is a scalar and, since the total expression on the left has been proved to be a scalar, the first term on the right is also a scalar, and $A^i - (1/2)g^{-1/2}\partial(g^{1/2}B^{ij})/\partial z^j$ a contravariant vector. Conversely, Graham's proof could be used as a starting point to verify the contravariant vector character of $A^i + \Gamma^i_{kl}B^{kl}/2$.

Both contravariant combinations are useful, $A^i + \Gamma^i_{kl}B^{kl}/2$ leads to an easy derivation of the standard form of the Fokker-Planck equations whereas Graham's combination leads in a natural way to the so-called Stratonovich form [9] of the Fokker-Planck equation.

Drift and diffusion contributions to the right of (4) are rearranged according to (18). Volume, inner contributions are considered first; scalar weights (with dV) are considered instead of probabilities (with $d^M z$) to preserve manifest covariance

$$\begin{aligned}
&\left(A^i\frac{\partial f}{\partial z^i} + \frac{1}{2}B^{ij}\frac{\partial^2 f}{\partial z^i\partial z^j}\right)\overline{P^+}\\
&= \left[\left(A^i + \frac{B^{kl}}{2}\Gamma^i_{kl}\right)f_{;i} + \frac{B^{ij}}{2}f_{;ij}\right]\overline{P^+}\\
&= \left[f\left(A^i + \frac{B^{kl}}{2}\Gamma^i_{kl}\right)\overline{P^+}\right]_{;i} - f\left[\left(A^i + \frac{B^{kl}}{2}\Gamma^i_{kl}\right)\overline{P^+}\right]_{;i} + \frac{1}{2}\left(B^{ji}\overline{P^+}f_{;j}\right)_{;i}\\
&\quad - \frac{1}{2}\left[\left(B^{ij}\overline{P^+}\right)_{;j}f\right]_{;i} + \frac{f}{2}\left(B^{ij}\overline{P^+}\right)_{;ji} = \left[f\left(A^i\overline{P^+} - \frac{1}{2g^{1/2}}\frac{\partial B^{ij}\overline{P^+}g^{1/2}}{\partial z^j}\right)\right.\\
&\quad \left. + f_{;j}\frac{B^{ji}}{2}\overline{P^+}\right]_{;i} - \frac{f}{g^{1/2}}\left(\frac{\partial A^i\overline{P^+}g^{1/2}}{\partial z^i} - \frac{1}{2}\frac{\partial^2 B^{ij}\overline{P^+}g^{1/2}}{\partial z^i\partial z^j}\right)
\end{aligned} \tag{22}$$

where mute indices have been freely renamed and the symmetric character of B^{ij}, check its definition in (7), applied if needed. The chain rule and the rule for the divergence of a vector, $V^i_{;i} = g^{-1/2}\partial V^i g^{1/2}/\partial z^i$, and of a second-order tensor, $T^{ij}_{;j} = g^{-1/2}\partial T^{ij}g^{1/2}/\partial z^j + \Gamma^i_{kl}T^{kl}$, have been used. After applying a volume integral to (22), the expression of change of the global PDF (with possible singular contributions) due to the evolution of its inner contribution is obtained. This expression is valid in G and in G_1 and, as it happened with the inertial contribution, there is a contribution from both of them to the singularity at S with opposite sign.

$$
\begin{aligned}
&\int \frac{f}{g^{1/2}}\Big(\frac{1}{2}\frac{\partial^2 B^{ij}\overline{P^+}g^{1/2}}{\partial z^i \partial z^j} - \frac{\partial A^i \overline{P^+} g^{1/2}}{\partial z^i}\Big)\,dV \\
&\quad - \oint f\left[A^n\overline{P^+} - \frac{1}{2g^{1/2}}\frac{\partial B^{nj}\overline{P^+}g^{1/2}}{\partial z^j}\right]^S dS - \oint \frac{\partial f}{\partial z^j}\Big[\frac{B^{jn}}{2}\overline{P^+}\Big]^S dS \\
&\quad = \int f\Big(\frac{1}{2}\frac{\partial^2 B^{ij}P^+}{\partial z^i\partial z^j} - \frac{\partial A^i P^+}{\partial z^i}\Big)\,d^M z + \oint f\left(\left[\frac{1}{2}\frac{\partial B^{nj}P^+}{\partial z^j} - A^n P^+\right]^S \frac{a^{1/2}}{g^{1/2}}\right. \\
&\quad\quad \left. + \frac{1}{2}\frac{\partial (a/g)^{1/2}[B^{\alpha n}P^+]^S}{\partial \zeta^\alpha}\right) d^{M-1}\zeta - \oint \frac{\partial f}{\partial z^{(n)}}\Big[\frac{B^{(n)(n)}}{2}P^+\Big]^S \frac{a^{1/2}}{g^{1/2}}\,d^{M-1}\zeta
\end{aligned} \tag{23}
$$

where index n has been used to indicate a component normal to S and it has been assumed that the metrics of the full phase space $\mathbb{R}^M$ has no discontinuities at S, though its derivative parallel to S is not necessarily zero. The last term of the first expression has been expanded in the second equality by isolating the derivative of the test function normal to S, using the chain rule for the components parallel to S (when computing surface quantities, work is assumed to be in a coordinate system with $M-1$ components locally parallel to S at S plus one component normal to S at S) and applying the divergence theorem on a closed surface what yields a zero contribution since the boundary of a boundary is the empty set [18]. As in the inertial term, $[W]^S$ means a difference between the value of W in the limit as G_1 approaches a point in S and the limit at the same point coming from G, $[W]^S = (W_{G1} - W_G)|_S$.

Next, drift and diffusion are rearranged according to (21). An expression similar to (22) is obtained for the volume contribution

$$
\begin{aligned}
&\Big(A^i\frac{\partial f}{\partial z^i} + \frac{1}{2}B^{ij}\frac{\partial^2 f}{\partial z^i\partial z^j}\Big)\overline{P^+} \\
&\quad = \Big[\overline{A}^i f_{;i} + \frac{1}{2}(B^{ij}f_{;i})_{;j}\Big]\overline{P^+} \\
&\quad = (f\overline{A}^i\overline{P^+})_{;i} - f(\overline{A}^i\overline{P^+})_{;i} + \frac{1}{2}[(f_{;i}B^{ij}\overline{P^+})_{;j} - (fB^{ij}\overline{P^+}_{;j})_{;i} + f(B^{ij}\overline{P^+}_{;j})_{;i}] \\
&\quad = \Big[f(\overline{A}^i\overline{P^+} - \frac{B^{ij}}{2}\overline{P^+}_{;j}) + f_{;j}\frac{B^{ji}}{2}\overline{P^+}\Big]_{;i} - f\big(\overline{A}^i\overline{P^+} - (B^{ij}/2)\overline{P^+}_{;j}\big)_{;i}
\end{aligned} \tag{24}
$$

where $\overline{A}^i$ is a short-hand notation for the contravariant vector $A^i - g^{-1/2}\partial((B^{ij}/2)g^{1/2})/\partial z^j$. The same considerations leading from (22) to (23) are applied to (24) in order to obtain the equivalent of (23)

$$
\begin{aligned}
&\int f\Big[\Big(\frac{B^{ij}}{2}\overline{P^+}_{;j}\Big)_{;i} - (\overline{A}^i\overline{P^+})_{;i}\Big]dV + \oint\Big\{f\Big[\frac{B^{nj}}{2}\overline{P^+}_{;j} - \overline{A}^n\overline{P^+}\Big]^S - f_{;j}\Big[\frac{B^{jn}}{2}\overline{P^+}\Big]^S\Big\}dS \\
&= \int f\Big[\Big(\frac{B^{ij}}{2}\overline{P^+}_{;j}\Big)_{;i} - (\overline{A}^i\overline{P^+})_{;i}\Big]dV + \oint f\Big(\Big[\frac{B^{nj}}{2}\overline{P^+}_{;j} - \overline{A}^n\overline{P^+}\Big]^S
\end{aligned}
$$

$$+\frac{1}{2}[B^{\alpha n}\overline{P^{+}}]^{S}_{;\alpha}\Big)\,dS-\oint\frac{\partial f}{\partial z^{(n)}}\Big[\frac{B^{(n)(n)}}{2}\overline{P^{+}}\Big]^{S}dS$$
$$=\int f\Big[\Big(\frac{B^{ij}}{2}\overline{P^{+}}_{;j}\Big)_{;i}-(\overline{A}^{i}\overline{P^{+}})_{;i}\Big]dV+\int f\Big(\Big[\frac{B^{nj}}{2}\overline{P^{+}}_{;j}-\overline{A}^{n}\overline{P^{+}}\Big]^{S}$$
$$+\frac{1}{2}[B^{\alpha n}\overline{P^{+}}]^{S}_{;\alpha}\Big)\delta_S\,dV+\int f\frac{\partial}{\partial z^{(n)}}\Big(\Big[\frac{B^{(n)(n)}}{2}\overline{P^{+}}\Big]^{S}\delta_S\Big)\,dV \tag{25}$$

with an explicit use of singularities at the boundaries with volume integrals instead of surface integrals. Equations (23) and (25) may be proved to be identical [20].

Now, the explicit singular contribution to diffusion and drift is analysed. In the derivation of a term analogous to (22) some care is needed: derivatives of the test function in a direction normal to S must be isolated. This task is performed straightforwardly by going back to the integrand on the right of (4). Generic coordinate changes are now those which modify surface coordinates leaving unmodified the component normal to the surface. Under this restriction, both $\partial f/\partial z^n$ and $\partial^2 f/\partial z^{n2}$ behave as scalar fields defined on the surface S, whereas $\partial^2 f/\partial\zeta^\alpha z^n$ is a covector defined on S with regard to the index α ($\partial z^i/\partial z'^n=\delta^i_n$ when only coordinates parallel to S are modified). The expression equivalent to (18) reads now

$$\Big(A^{\alpha}+\frac{B^{\beta\delta}}{2}\Gamma^{\alpha}_{\beta\delta}\Big)f_{;\alpha}+\frac{B^{\beta\delta}}{2}f_{;\beta\delta}+A^{(n)}\frac{\partial f}{\partial z^{(n)}}+\frac{B^{(n)(n)}}{2}\frac{\partial^2 f}{\partial z^{(n)2}}+B^{(n)\alpha}\frac{\partial^2 f}{\partial z^{(n)}\partial\zeta^{\alpha}} \tag{26}$$

where use has been made of the symmetry of B^{ij}. The expression equivalent to (21) is

$$\Big(A^{\alpha}-\frac{1}{a^{1/2}}\frac{\partial a^{1/2}(B^{\alpha\beta}/2)}{\partial\zeta^{\beta}}\Big)f_{;\alpha}+\Big(\frac{B^{\alpha\beta}}{2}f_{;\alpha}\Big)_{;\beta}+A^{(n)}\frac{\partial f}{\partial z^{(n)}}$$
$$+\frac{B^{(n)(n)}}{2}\frac{\partial^2 f}{\partial z^{(n)2}}+B^{(n)\alpha}\frac{\partial^2 f}{\partial z^{(n)}\partial\zeta^{\alpha}} \tag{27}$$

The derivation of the surface equations similar to (22) and (24) follows the same lines. The only difference is that the determinant of the metrics is now a and the presence of normal derivatives of the test function which are equivalent to layer generalised functions defined on S; the chain rule is applied to the last term of (26) and (27).

$$\Big[f\Big(A^{\alpha}\gamma_S-\frac{1}{2a^{1/2}}\frac{\partial B^{\alpha\beta}\gamma_S a^{1/2}}{\partial\zeta^{\beta}}\Big)+f_{;\beta}\frac{B^{\beta\alpha}}{2}\gamma_S\Big]_{;\alpha}$$
$$-\frac{f}{a^{1/2}}\Big(\frac{\partial A^{\alpha}\gamma_S a^{1/2}}{\partial\zeta^{\alpha}}-\frac{1}{2}\frac{\partial^2 B^{\alpha\beta}\gamma_S a1/2}{\partial\zeta^{\alpha}\partial\zeta^{\beta}}\Big)$$
$$+\gamma_S A^{(n)}\frac{\partial f}{\partial z^{(n)}}+\gamma_S\frac{B^{(n)(n)}}{2}\frac{\partial^2 f}{\partial z^{(n)2}}+\Big(\gamma_S B^{(n)\alpha}\frac{\partial f}{\partial z^{(n)}}\Big)_{;\alpha}-(\gamma_S B^{(n)\alpha})_{;\alpha}\frac{\partial f}{\partial z^{(n)}} \tag{28}$$
$$\Big[f\big(\overline{A}^{\alpha}_{S}\gamma_S-\frac{B^{\alpha\beta}}{2}\gamma_{S;\beta}\big)+f_{;\beta}\frac{B^{\beta\alpha}}{2}\gamma_S\Big]_{;\alpha}-f\big(\overline{A}^{\alpha}_{S}\gamma_S-\frac{B^{\alpha\beta}}{2}\gamma_{S;\beta}\big)_{;\alpha}+\gamma_S A^{(n)}\frac{\partial f}{\partial z^{(n)}}$$
$$+\gamma_S\frac{B^{(n)(n)}}{2}\frac{\partial^2 f}{\partial z^{(n)2}}+\Big(\gamma_S B^{(n)\alpha}\frac{\partial f}{\partial z^{(n)}}\Big)_{;\alpha}-(\gamma_S B^{(n)\alpha})_{;\alpha}\frac{\partial f}{\partial z^{(n)}} \tag{29}$$

where $\overline{A}^{\alpha}_{S}$ is now Graham's vector on a surface $A^{\alpha}-a^{-1/2}\partial((B^{\alpha\beta}/2)a^{1/2})/\partial\zeta^{\beta}$.

Since the final result must be integrated over a closed surface, a boundary manifold without boundaries itself, pure surface divergence terms will have a zero integral contribution. The expressions equivalent to (23) and (25) read

$$\oint f\Big(\frac{1}{2}\frac{\partial^2 B^{\alpha\beta}P_S}{\partial\zeta^\alpha\partial\zeta^\beta}-\frac{\partial A^\alpha P_S}{\partial\zeta^\alpha}\Big)d^{M-1}\zeta+\oint\frac{\partial f}{\partial z^{(n)}}\Big(A^{(n)}P_S-\frac{\partial B^{(n)\alpha}P_S}{\partial\zeta^\alpha}\Big)d^{M-1}\zeta$$
$$+\oint\frac{\partial^2 f}{\partial z^{(n)2}}P_S\frac{B^{(n)(n)}}{2}d^{M-1}\zeta \tag{30}$$

$$\int f\Big[\Big(\frac{B^{\alpha\beta}}{2}\gamma_{S;\beta}\Big)_{;\alpha}-(\overline{A}^\alpha_S\gamma_S)_{;\alpha}\Big]\delta_S\,dV-\int f\frac{\partial}{\partial z^{(n)}}\Big[\Big(A^{(n)}\gamma_S-(B^{(n)\alpha}\gamma_S)_{;\alpha}\Big)\delta_S\Big]dV$$
$$+\int f\frac{\partial^2}{\partial z^{(n)2}}\Big(\gamma_S\frac{B^{(n)(n)}}{2}\delta_S\Big)dV \tag{31}$$

where there are no contributions from either G or G_1, since the previous expressions are intrinsic to S. It should be remembered [16] that the exact value of drift and diffusion coefficients on the surface may be different from their limits, as S is approached, inside either G or G_1. In (31), the triple layer functional has been defined by

$$\oint\nu\frac{\partial^2 f}{\partial n^2}dS=\int f\frac{\partial^2(\nu\delta_S)}{\partial n^2}dV$$

Now, the global drift plus diffusion contribution may be written down in two different ways. In the first one, (23) and (30) are added to yield (32); (25) plus (31) lead to (33) which is the second option

$$\int f\Big(\frac{1}{2}\frac{\partial^2 B^{ij}P^+}{\partial z^i\partial z^j}-\frac{\partial A^i P^+}{\partial z^i}\Big)d^M z+\oint f\Bigg(\frac{1}{2}\frac{\partial^2 B_S^{\alpha\beta}P_S}{\partial\zeta^\alpha\partial\zeta^\beta}-\frac{\partial A_S^\alpha P_S}{\partial\zeta^\alpha}$$
$$+\Big[\frac{1}{2}\frac{\partial B^{nj}P^+}{\partial z^j}-A^n P^+\Big]^S\frac{a^{1/2}}{g^{1/2}}+\frac{1}{2}\frac{\partial(a/g)^{1/2}[B^{\alpha n}P^+]^S}{\partial\zeta^\alpha}\Bigg)d^{M-1}\zeta$$
$$+\oint\frac{\partial f}{\partial z^{(n)}}\Big(A_S^{(n)}P_S-\frac{\partial B_S^{(n)\alpha}P_S}{\partial\zeta^\alpha}-\Big[\frac{B^{(n)(n)}}{2}P^+\Big]^S\frac{a^{1/2}}{g^{1/2}}\Big)d^{M-1}\zeta$$
$$+\oint\frac{\partial^2 f}{\partial z^{(n)2}}\frac{B_S^{(n)(n)}}{2}P_S\,d^{M-1}\zeta \tag{32}$$

$$\int f\Big[\frac{B^{ij}}{2}\overline{P^+}_{;j}-\overline{A}^i\overline{P^+}\Big]_{;i}dV+\int f\Bigg(\Big(\frac{B_S^{\alpha\beta}}{2}\gamma_{S;\beta}-\overline{A}^\alpha_S\gamma_S\Big)_{;\alpha}$$
$$+\Big[\frac{B^{nj}}{2}\overline{P^+}_{;j}-\overline{A}^n\overline{P^+}\Big]^S+\frac{1}{2}[B^{\alpha n}\overline{P^+}]^S_{;\alpha}\Bigg)\delta_S\,dV+\int f\frac{\partial}{\partial z^{(n)}}\Big\{\Big[(B_S^{(n)\alpha}\gamma_S)_{;\alpha}$$
$$-A_S^{(n)}\gamma_S+\Big[\frac{B^{(n)(n)}}{2}\overline{P^+}\Big]^S\Big]\delta_S\Big\}dV+\int f\frac{\partial^2}{\partial z^{(n)2}}\Big(\gamma_S\frac{B^{(n)(n)}}{2}\delta_S\Big)dV \tag{33}$$

In (32) and (33) a subindex S has been added to drift and diffusion coefficients computed on S since a discontinuity in their values at the boundary is not excluded. The term $(B_S^{(n)\alpha}\gamma_S)_{;\alpha}-A_S^{(n)}\gamma_S$ in (33) could be rewritten as $(B_S^{(n)\alpha}\gamma_S/2)_{;\alpha}+(B_S^{(n)\alpha}/2)\gamma_{S;\alpha}-\overline{A}_S^{(n)}\gamma_S$.

3.3 Jump Term

The last contribution to (4) is the jump term.

$$\int f(z)\left\{\fint \left[W(z|\boldsymbol{x};t)P(\boldsymbol{x};t) - W(\boldsymbol{x}|z;t)P(z;t)\right] d^M x\right\} d^M z \tag{34}$$

where P and W are PDF's: the first one is the PDF of being somewhere in the phase space and the second one is the PDF of jumping to another point, conditional on being at the original point. Equation (34) may be expressed in terms of scalar weights instead of PDF's

$$\int f(z)\left\{\fint \left[\overline{W}(z|\boldsymbol{x};t)\overline{P}(\boldsymbol{x};t) - \overline{W}(\boldsymbol{x}|z;t)\overline{P}(z;t)\right] d_x V\right\} d_z V \tag{35}$$

With either a PDF or a scalar weight form, both P, $\overline{P}$ and W, $\overline{W}$ have to be decomposed into volume and surface contributions. If the final point lies in S, W and $\overline{W}$ are of the singular surface type: W_S defined on S and $\gamma_W \delta_S$, respectively; if the original point lies in S, P and $\overline{P}$ are of the singular surface type: P_S defined on S and $\gamma_S \delta_S$, respectively.

The full phase space comprises $G \cup S \cup G_1$; so, there are nine basic sorts of jump to consider: $G \to G$, $G \to S$, $G \to G_1$, $S \to G$, $S \to S$, $S \to G_1$, $G_1 \to G$, $G_1 \to S$ and $G_1 \to G_1$. Since G_1 acts as an external reservoir, $G_1 \to G_1$ processes are irrelevant from the point of view of studying what occurs in $\overline{G}$. On the other hand, the fine-grained detail of where in G_1 a particle jumps from either G or S is irrelevant, too; it only matters the global integral probability of any jump to an inner point of G_1 as a death process, $\mathfrak{D}(z;t) = \fint_{G1} W(\boldsymbol{x}|z;t)\, d^M x = \fint_{G1} \overline{W}(\boldsymbol{x}|z;t)\, d_x V = \overline{\mathfrak{D}}(z;t)$. In its turn, the fine-grained detail of where in G_1 is a particle jumping from, into either G or S, is also irrelevant it only matters the global integral probability of any jump from an inner point of G_1 as a birth process, $\mathfrak{B}(z;t) = \fint_{G1} W(z|\boldsymbol{x};t)P(\boldsymbol{x};t)\, d^M x = \fint_{G1} W(z|\boldsymbol{x};t)\overline{P}(\boldsymbol{x};t)\, d_x V = g^{1/2}\overline{\mathfrak{B}}(z;t) = g^{1/2}(z)\fint_{G1} \overline{W}(z|\boldsymbol{x};t)\overline{P}(\boldsymbol{x};t) d_x V$. The previous definitions of death and birth processes assume that the PDF in G_1 is normalized; anyway, these integral definitions are possible physical interpretations, which make the whole formulation consistent in terms of the only relevant values: the final death and birth rates regardless of how is P in G_1. Any reference to G_1 could have been supressed and one could have assumed that, apart from jumps inside $\overline{G}$, there were also death and birth processes with given rates.

The details of the origin and end of jumps in (34) may be explicitly stated

$$\begin{aligned}
&\int_G f(z)\left\{\fint_G \left[W(z|\boldsymbol{x};t)P^+(\boldsymbol{x};t) - W(\boldsymbol{x}|z;t)P^+(z;t)\right] d^M x\right\} d^M z \\
&\quad + \int_S f(\boldsymbol{\zeta})\left\{\fint_G \left[W_S(\boldsymbol{\zeta}|\boldsymbol{x};t)P^+(\boldsymbol{x};t) - W(\boldsymbol{x}|\boldsymbol{\zeta};t)P_S(\boldsymbol{\zeta};t)\right] d^M x\right\} d^{M-1}\zeta \\
&\quad + \int_G f(z)\left\{\fint_S \left[W(z|\boldsymbol{\xi};t)P_S(\boldsymbol{\xi};t) - W_S(\boldsymbol{\xi}|z;t)P^+(z;t)\right] d^{M-1}\xi\right\} d^M z \\
&\quad + \int_S f(\boldsymbol{\zeta})\left\{\fint_S \left[W_S(\boldsymbol{\zeta}|\boldsymbol{\xi};t)P_S(\boldsymbol{\xi};t) - W_S(\boldsymbol{\xi}|\boldsymbol{\zeta};t)P_S(\boldsymbol{\zeta};t)\right] d^{M-1}\xi\right\} d^{M-1}\zeta \\
&\quad + \int_G f(z)\left[\mathfrak{B}_G(z;t) - \mathfrak{D}_G(z;t)P^+(z;t)\right] d^M z \\
&\quad + \int_S f(\boldsymbol{\zeta})\left[\mathfrak{B}_S(\boldsymbol{\zeta};t) - \mathfrak{D}_S(\boldsymbol{\zeta};t)P_S(\boldsymbol{\zeta};t)\right] d^{M-1}\zeta
\end{aligned} \tag{36}$$

where the first line represents $G \to G$ jumps, the second line represents the variation in singular PDF at S due to jumps $G \to S$ (increase) and $S \to G$ (decrease), the third line represents the variation in volume PDF at G due to jumps $S \to G$ (increase) and $G \to S$ (decrease), the fourth line represents $S \to S$ jumps, the fifth line birth and death processes in G, and the sixth line birth and death processes in S.

An expression equivalent to (36) in terms of scalar weights reads

$$
\begin{aligned}
&\int f(z)\left\{⨍\left[\overline{W}(z|\boldsymbol{x};t)\overline{P^+}(\boldsymbol{x};t) - \overline{W}(\boldsymbol{x}|z;t)\overline{P^+}(z;t)\right]d_xV\right\}d_zV\\
&\quad+\int f(z)\left\{⨍\left[\gamma_W(z|\boldsymbol{x};t)\overline{P^+}(\boldsymbol{x};t) - \overline{W}(\boldsymbol{x}|z;t)\gamma_S(z;t)\right]d_xV\right\}\delta_S(z,t)\,d_zV\\
&\quad+\int f(z)\left\{⨍\left[\overline{W}(z|\boldsymbol{x};t)\gamma_S(\boldsymbol{x};t) - \gamma_W(\boldsymbol{x}|z;t)\overline{P^+}(z;t)\right]\delta_S(\boldsymbol{x},t)\,d_xV\right\}d_zV\\
&\quad+\int f(z)\left\{⨍\left[\gamma_W(z|\boldsymbol{x};t)\gamma_S(\boldsymbol{x};t) - \gamma_W(\boldsymbol{x}|z;t)\gamma_S(z;t)\right]\delta_S(\boldsymbol{x},t)\,d_xV\right\}\delta_S(z,t)\,d_zV\\
&\quad+\int f(z)\left[\overline{\mathfrak{B}_G}(z;t) - \mathfrak{D}_G(z;t)\overline{P^+}(z;t)\right]d_zV\\
&\quad+\int f(z)\left[\overline{\mathfrak{B}_S}(z;t) - \mathfrak{D}_S(z;t)\gamma_S(z;t)\right]\delta_S(z,t)\,d_zV
\end{aligned}
\tag{37}
$$

Were the boundary excluded from the domain, $G \to G$ plus death and birth processes would be the only relevant terms remaining. It means that second, third, fourth and sixth lines in (36) and (37) would be supressed, whereas death and birth rates would be modified to take into account what, previously, have been explicitly considered as $G \to S$ and $S \to G$ exchanges. Namely, the effect of lines two and three should be retained as modified death and birth rates in line five, whereas lines four and six would become irrelevant.

3.4 Gathering All Terms

The final PDF evolution equation is obtained by joining (14) (inertial term), (32) (drift plus diffusion terms) and (36) (jump term). After that, volume integrals are separated from surface integrals and the latter are further split according to the order of the normal derivative of the test function. Since test functions are free members of class C^2 in $\mathbb{R}^M$, the resulting integral equalities must be satisfied by the factors multiplying the test functions in the integrands and no assumption on the properties of f close to the boundary is made

$$
\begin{aligned}
\frac{\partial P^+}{\partial t} &= -\frac{\partial A^i P^+}{\partial z^i} + \frac{1}{2}\frac{\partial^2 B^{ij}P^+}{\partial z^i \partial z^j} + ⨍_G \left[W(z|\boldsymbol{x};t)P^+(\boldsymbol{x};t) - W(\boldsymbol{x}|z;t)P^+(z;t)\right]d^Mx\\
&\quad+ ⨍_S \left[W(z|\boldsymbol{\xi};t)P_S(\boldsymbol{\xi};t) - W_S(\boldsymbol{\xi}|z;t)P^+(z;t)\right]d^{M-1}\xi + \mathfrak{B}_G - \mathfrak{D}_G P^+
\end{aligned}
\tag{38}
$$

$$
\begin{aligned}
\frac{\partial P_S}{\partial t} &= -\frac{\partial A_S^\alpha P_S}{\partial \zeta^\alpha} + \frac{1}{2}\frac{\partial^2 B_S^{\alpha\beta}P_S}{\partial \zeta^\alpha \partial \zeta^\beta} + \left[\frac{1}{2}\frac{\partial B^{nj}P^+}{\partial z^j} + (\dot{z}_S^n - A^n)P^+\right]^S \frac{a^{1/2}}{g^{1/2}}\\
&\quad+ \frac{1}{2}\frac{\partial [B^{\alpha n}P^+]^S (a/g)^{1/2}}{\partial \zeta^\alpha} + ⨍_G \left[W_S(\boldsymbol{\zeta}|\boldsymbol{x};t)P^+(\boldsymbol{x};t) - W(\boldsymbol{x}|\boldsymbol{\zeta};t)P_S(\boldsymbol{\zeta};t)\right]d^Mx\\
&\quad+ ⨍_S \left[W_S(\boldsymbol{\zeta}|\boldsymbol{\xi};t)P_S(\boldsymbol{\xi};t) - W_S(\boldsymbol{\xi}|\boldsymbol{\zeta};t)P_S(\boldsymbol{\zeta};t)\right]d^{M-1}\xi + \mathfrak{B}_S - \mathfrak{D}_S P_S
\end{aligned}
\tag{39}
$$

$$\dot{z}_S^n P_S = A_S^n P_S - \frac{\partial B_S^{n\alpha} P_S}{\partial \zeta^\alpha} - \left[\frac{B^{(n)(n)}}{2} P^+\right]^S \frac{a^{1/2}}{g^{1/2}} \tag{40}$$

$$B_S^{(n)(n)} P_S = 0 \tag{41}$$

Equation (38) gives the evolution of the PDF in G, (39) gives the evolution of the singular contribution to the PDF in S, (40) and (41) are restrictions needed to guarantee that no generalised functions of order higher than the simple layer develop. In (39), it has been used the fact that the velocity of the boundary $\dot{z}_S^n$ has a unique value defined on S to make $\dot{z}_S^n [P^+]^S = \dot{z}_S^n (P_{G1}^+ - P_G^+) = [\dot{z}_S^n P^+]^S$.

The final scalar weight evolution equation may be obtained in a similar way from (13), (33) and (37)

$$\frac{\partial \overline{P^+}}{\partial t} = \left(\frac{B^{ij}}{2} \overline{P^+}_{;j} - \overline{A}^i \overline{P^+}\right)_{;i} + ⨍ \left[\overline{W}(z|\boldsymbol{x};t)\overline{P^+}(\boldsymbol{x};t) - \overline{W}(\boldsymbol{x}|z;t)\overline{P^+}(z;t)\right] d_x V$$
$$+ ⨍_S \left[\overline{W}(z|\boldsymbol{\xi};t)\gamma_S(\boldsymbol{\xi};t) - \gamma_W(\boldsymbol{\xi}|z;t)\overline{P^+}(z;t)\right] d_\xi S + \overline{\mathfrak{B}_G} - \mathfrak{D}_G \overline{P^+} \tag{42}$$

$$\frac{\partial \gamma_S}{\partial t} = -\frac{\gamma_S}{2a}\dot{a} + \left(\frac{B_S^{\alpha\beta}}{2}\gamma_{S;\beta} - \overline{A}_S^\alpha \gamma_S\right)_{;\alpha} + \left[\frac{B^{nj}}{2}\overline{P^+}_{;j} + (\dot{z}_S^n - \overline{A}^n)\overline{P^+}\right]^S$$
$$+ \frac{1}{2}[B^{\alpha n}\overline{P^+}]^S_{;\alpha} + ⨍ \left[\gamma_W(z|\boldsymbol{x};t)\overline{P^+}(\boldsymbol{x};t) - \overline{W}(\boldsymbol{x}|z;t)\gamma_S(z;t)\right] d_x V$$
$$+ ⨍_S \left[\gamma_W(z|\boldsymbol{\xi};t)\gamma_S(\boldsymbol{\xi};t) - \gamma_W(\boldsymbol{\xi}|z;t)\gamma_S(z;t)\right] d_\xi S + \overline{\mathfrak{B}_S} - \mathfrak{D}_S \gamma_S \tag{43}$$

$$\dot{z}_S^n \gamma_S = \overline{A}_S^n \gamma_S - (B_S^{n\alpha}\gamma_S/2)_{;\alpha} - (B_S^{n\alpha}/2)\gamma_{S;\alpha} - \left[\frac{B^{(n)(n)}}{2}\overline{P^+}\right]^S \tag{44}$$

$$B_S^{(n)(n)} \gamma_S = 0 \tag{45}$$

Equation (42) gives the evolution of the scalar weight field in G, (43) provides the evolution of the singular contribution to the scalar weight field in S, (44) and (45) pose restrictions equivalent to those of (40) and (41) to guarantee that there are neither double nor triple layer singularities, which cannot be normalized.

If probabilities were to be computed in G instead of $\overline{G}$, leaving S out of the previous analysis, the only relevant equations would be (38) and (42) without $G \to S$ and $S \to G$ jumps, the third term on the right in both cases. The reason is that, without S in the domain, values defined exactly at S such as γ_S and the discontinuities in volume flow properties may be assumed to be zero; whereas jumps involving S may be accounted as birth-death processes.

It is interesting to notice that probability currents (drift plus diffusion contributions) are defined inside G by means of $A^i P^+ - (1/2)\partial(B^{ij}P^+)/\partial z^j = \Phi^i$ for the standard set of equations and $\overline{A}^i \overline{P^+} - (1/2)B^{ij}\overline{P^+}_{;j} = \overline{\Phi}^i$ for the Stratonovich-like set. There is also an inertial probability current, in the case of moving boundaries, defined by either $\dot{z}_S^n P^+$ or $\dot{z}_S^n \overline{P^+}$. The use of these probability currents allows for a more compact writing of the previous sets of PDF evolution equations.

3.5 Renormalization

From (3), it should be satisfied

$$\frac{d}{dt}\left[\int P^{+}\,dV + \oint \gamma_S\,dS\right] = 0 \tag{46}$$

Recalling the computation of the inertial contribution, the previous expression may be transformed into

$$\int \frac{\partial P^{+}}{\partial t}\,dV + \oint\left\{\frac{\partial \gamma_S}{\partial t} + \frac{\gamma_s}{a^{1/2}}\frac{\partial a^{1/2}}{\partial t} + \dot{z}^n_S\overline{P^{+}}_G\right\}dS = \dot{W}_N = 0 \tag{47}$$

where W_N is the normalized global weight which should be unity and $\dot{W}_N$ its time derivative.

Equations (42) and (43) are substituted into (47) and the divergence theorem is applied, remembering that its application in S yields a zero contribution. Most terms cancel each other, jump terms, divergences in S and the divergence in G, with the boundary value as S is approached from inside G. However, there are some terms remaining,

$$\begin{aligned}\dot{W}_N = &\oint\left(\frac{B^{nj}_{G1}}{2}\overline{P^{+}_{G1;j}} + (\dot{z}^n_S - \overline{A}^n_{G1})\overline{P^{+}_{G1}}\right)dS + \int(\overline{\mathfrak{B}_G} - \mathfrak{D}_G\overline{P^{+}})\,dV\\ &+ \oint(\overline{\mathfrak{B}_S} - \mathfrak{D}_S\gamma_S)\,dS\end{aligned} \tag{48}$$

corresponding to the global probability flow, inertial, drift and diffusion, from the external region, G_1, to the inner one, G, plus the global balance between birth and death processes. $\dot{W}_N$, according to (48), could be different from zero; this problem may be solved [21] adding a term proportional to $\overline{P}$ or P (depending on whether scalar weights of PDF's are used) to compensate it.

$-\dot{W}_N P^{+}$ should be added to the right of (38), $-\dot{W}_N P_S$ to the right of (39), $-\dot{W}_N\overline{P^{+}}$ to the right of (42) and $-\dot{W}_N\gamma_S$ to the right of (43) when there is some net flow of probability inward or outward of the studied zone.

It is interesting to notice that $\dot{W}_N$ is hardly affected by including or excluding S in the domain: instead of variables evaluated as G_1 approaches S, there will be variables computed as G approaches S and birth-death processes at S stop being considered. Anyway, if S is out of the domain, there is no point in making a difference between approaching S from G and approaching S from G_1; $X_{G1} = X_G = X_S$ could be assumed for any volume property X. Instead of (48), the renormalization would be given by

$$\dot{W}_N = \oint\left(\frac{B^{nj}_G}{2}\overline{P^{+}_{G;j}} + (\dot{z}^n_S - \overline{A}^n_G)\overline{P^{+}_G}\right)dS + \int(\overline{\mathfrak{B}_G} - \mathfrak{D}_G\overline{P^{+}})\,dV \tag{49}$$

namely, the divergence term in G, as there are no surface terms at the boundary to cancel it, plus the global birth-death balance in the inner region.

4 Physical Interpretation

Equations (38) and (42) represent standard differential Chapman-Kolmogorov equations [9] defined inside an open M dimensional manifold, $G \in \mathbb{R}^M$, with the possibility of having birth-death processes and jumps from and into a possible singularity at the boundary. The first equation is in the standard form, whereas the second one is in the Stratonovich form. Its integration by means of Monte Carlo processes is well known [9, 20] in terms of Stochastic Differential Equations (SDE) equivalent to the partial differential terms on the right, drift plus diffusion, which define random paths for each Monte Carlo particle punctuated with jumps, discontinuities in the path, whose amplitude and frequency of occurrence has a probability given by the integral terms on the right. Birth processes appear as paths starting from scratch inside G, whereas death processes are represented by paths ending inside G. The presence of a subspace $G_1 = \mathbb{R}^M \backslash \overline{G}$, considered as an external probability reservoir, allows for a physical picture of birth-death processes as a special kind of jumps from and into G_1. Jumps from or into the boundary S, $⨏_S \big[W(z|\boldsymbol{\xi};t)P_S(\boldsymbol{\xi};t) - W_S(\boldsymbol{\xi}|z;t)P^+(z;t)\big]\,d^{M-1}\xi$ in (38) or the equivalent term in (42), have a correlate with opposite sign in the evolution of the singular probability restricted to S, $⨏_G \big[W_S(\boldsymbol{\zeta}|\boldsymbol{x};t)P^+(\boldsymbol{x};t) - W(\boldsymbol{x}|\boldsymbol{\zeta};t)P_S(\boldsymbol{\zeta};t)\big]\,d^M x$ in (39) or the equivalent term in (43). This means that jumps $G \to S$ and $S \to G$ are just redistribution terms which do not affect the global integral probability weight. Were there neither jumps nor birth-death processes, the usual Fokker-Planck equations would be recovered. Fokker-Planck equations restricted to the particular case with no diffusion are Liouville equations. Were there neither diffusion, nor drift, the corresponding particular case would be that of Master equations.

Equations (39) and (43) provide with the evolution of either the PDF or the scalar weight inside the boundary of G defined as a closed, $M-1$, piecewise, smooth manifold. In a Monte Carlo picture, a singularity at a $M-1$ manifold shows as a set of particles whose movement has some restriction which favours new positions inside that manifold; not surprisingly, terms equivalents to those defined in G are found in S: there are birth-death, inner jumps, drift and diffusion terms with the same form as those defined in G but restricted to positions inside S. The use of intrinsic surface coordinates would permit Monte Carlo particles moving inside S in a natural way. Aside from that, there are also exchange terms between S and G plus the effect of a possible deformation of S in its intrinsic metrics determinant. This last contribution only shows explicitly when the equation is expressed in terms of a scalar weight surface function; when the equation is expressed in terms of a surface PDF, the determinant metrics is included in the PDF. Exchange terms, in their turn, are easily classified in three classes:

(i) The reverse of the effect of $G \to S$ and $S \to G$ jumps. Reverse effect with regard to the same contribution to the probability inside G. What is lost by G is won by S and viceversa.
(ii) Probability currents normal to S which may come from either G or G_1. The effect of a moving boundary, steming from the inertial term, is included here if present, so that the only relevant probability currents with regard to singularity creation or depletion are those relative to the movement of the boundary.
(iii) An additional contribution from the crossed diffusion between diffusive transport parallel to S and diffusive transport normal to it, $(1/2)\partial\{[B^{\alpha n}P^+]^S(a/g)^{1/2}\}/\partial\zeta^\alpha$ in (39) or $(1/2)[B^{\alpha n}\overline{P^+}]^S_{;\alpha}$ in (43). This exchange contribution is zero in the important particular case that the diffusion tensor is diagonal.

All the exchange contributions are balanced: what is won in one side, is lost in another side when the full $\mathbb{R}^M = G \cup S \cup G_1$ is studied.

Exchange terms are more naturally expressed in terms of scalar weights, see (43), than in terms of PDF's, see (39) where the square root of the ratio of the determinant of the metrics in S and $\mathbb{R}^M$, $(a/g)^{1/2}$, appears in all of them. The reason being that, in both formulations, these exchange terms must be the same, whereas currents are more naturally expressed in a manifest covariant formulation. It is straightforward to check that

$$[B^{\alpha n}\overline{P^+}]^S_{;\alpha} dS = \frac{1}{a^{1/2}} \frac{\partial [B^{\alpha n}\overline{P^+} a^{1/2}]^S}{\partial \zeta^\alpha} a^{1/2} d^{M-1}\zeta = \frac{\partial [B^{\alpha n} P^+]^S (a/g)^{1/2}}{\partial \zeta^\alpha} d^{M-1}\zeta$$

$$\left[\overline{\Phi}^n\right]^S dS = \left[A^n \frac{P^+}{g^{1/2}} - \frac{B^{nj}}{2}\frac{\partial \overline{P^+}}{\partial z^j} - \frac{\overline{P^+}}{2g^{1/2}}\frac{\partial B^{nj} g^{1/2}}{\partial z^j}\right]^S a^{1/2} d^{M-1}\zeta$$
$$= \left[-\frac{1}{2}\frac{\partial B^{nj} P^+}{\partial z^j} + A^n P^+\right]^S \frac{a^{1/2}}{g^{1/2}} d^{M-1}\zeta = \left[\Phi^n\right]^S \frac{a^{1/2}}{g^{1/2}} d^{M-1}\zeta$$

where the first term on the left in both expressions corresponds to exchange terms in (43) and the last term on the right corresponds to the equivalent exchange term in (39). In the second derivation, it has been used the definition of $\overline{A}^i$ in terms of A^i, B^{ij} and $g^{1/2}$ and that of $P^+ = \overline{P^+} g^{1/2}$. In both expressions, it has been assumed that the metrics is continuous everywhere.

A better physical insight may be obtained by considering a Monte Carlo (particle) integration method: the behaviour of Monte Carlo particles at the boundary may be related to that of a light beam: it is either transmitted through the boundary, or absorbed by it, or emitted from it, or reflected. $-[\dot{z}^n_S + \overline{\Phi}^n]^S = k^n \neq 0$ means that there is a singularity at the boundary, that a non-zero surface integral value of $-(\dot{z}^n_S + \overline{\Phi}^n)_{G1}$ would require a renormalization of the PDF and that, depending on the sign, there is either a k^n probability current absorbed by the boundary or emitted from it. The value of $-(\dot{z}^n_S + \overline{\Phi}^n)_{G1}$ would provide the transmission in either sense according to its sign. On the other hand, $k^n = 0$ is compatible with either the presence of a previously created singularity which does not interact with the non-singular component, or with the absence of singularities. Anyway, either $-(\dot{z}^n_S + \overline{\Phi}^n)_G$ and $-(\dot{z}^n_S + \overline{\Phi}^n)_{G1}$ are both zero or are both equal and different from zero. Both values equal to zero mean that there is no probability current through the boundary which is either a natural, unattainable boundary [12] (particles would take an infinite time to reach it) or a regular boundary [12] with perfect reflection. Both values equal and different from zero are, in their turn, related to either an exit-absorbing or an entrance boundary condition [12] depending on the sign: particles either reach the limit and disappear there because of transmission into G_1 or come from G_1 and propagate into G. A regular boundary condition with partial reflection would be related to a finite, non-zero value of $-(\dot{z}^n_S + \overline{\Phi}^n)_G$ and $-(\dot{z}^n_S + \overline{\Phi}^n)_{G1}$ which should be matched by the fraction of particles being either absorbed/emitted or transmitted. It should be noticed that the difference between absorption at S and transmission into G_1 or between emission at S and transmission from G_1 is a matter of the physical picture chosen to explain the behaviour at the boundary. It could also be said that, whereas absorption/emission are related to interactions with a singularity at S, transmission is related to deletion/creation of particles at the boundary, that is to say, to a birth-death process at S, without involving any reference to an external probability reservoir at G_1.

The restriction given by (41) or (45) imply that the presence of a singularity at the boundary is incompatible with a non-zero value of the diffusion normal to the boundary, at the boundary. Either $P_S = \gamma_S a^{1/2}$, or $B_S^{(n)(n)}$, or both of them are zero. In a Monte Carlo method, it is immediate to realise that, were such a situation to appear (for instance as an initial condition), the diffusion process, which is random and normal to the singularity, would wear it out in one time step.

The restriction implied by (40) or (44) is more interesting. It is related to the possible movement of a singular boundary due to a non-zero probability current, normal to the boundary and defined at the boundary, plus an extra contribution from cross diffusion transport between coordinates parallel to S and normal to it, plus a contribution from a possible discontinuity in normal diffusion between G and G_1 at S. Notice that, whereas a non-zero normal diffusion at S is incompatible with a singularity at S, a non-zero normal drift (probability current) is not. In a Monte Carlo method, the first one transferred all the particles inside S to new random positions which could not define a new singularity, whereas the second one implies an ordinary and regular movement of all the particles inside S in a way which, at most, implies a deformation of S. The extra cross contribution has the same nature and may be thought of as an extra drift which comes from gradients parallel to S of cross diffusion between coordinates parallel to S and normal to it. However, the contribution from the discontinuity in normal diffusion at S is closely related to exchange terms in (39) and (43) and could be present even if there were no singularity at S. Of course, in such a situation a non-zero $[B^{(n)(n)}P^+]^S$ would imply the appearance of a non-integrable, double-layer singularity at the boundary, and therefore, it should be zero. In a Monte Carlo method, the solution accommodates itself with this restriction in a natural way. If there is a singularity and a non-zero discontinuity $[B^{(n)(n)}P^+]^S$, the singularity starts moving. If there is not a singularity and $[B^{(n)(n)}P^+]^S \neq 0$, a gradient in $B^{(n)(n)}P^+$ (no matter its stiffness) develops close to S so that $[B^{(n)(n)}P^+]^S = 0$ in the next time step. Diffusion moves particles between the G and the G_1 regions by a Wiener process, so that in the contact zone intermediate values between those typical of G and of G_1 develop instantly and these values may be extrapolated to fit the condition $[B^{(n)(n)}P^+]^S = 0$.

Although, $[B^{(n)(n)}P^+]^S = 0$, there are some differences between the situation where $(B^{(n)(n)}P^+)_G$ and $(B^{(n)(n)}P^+)_{G1}$ are both equal and different from zero and the situation where both are equal to zero. A non-zero value implies that there are particles reaching the boundary and being reflected at it (regular boundary condition [12]), whereas a zero value is related to either unattainable boundary condition (natural or entrance [12]) or to the absence of reflection (exit-trap-absorbing boundary condition [12]). In effect, let us assume that there is a non-zero value of $(B^{(n)(n)}P^+)_G$ and that an Euler, weak scheme [14] is used to integrate the corresponding SDE in a Monte Carlo method. Under those assumptions, half the particles at a distance from the boundary less than $\sqrt{B^{(n)(n)}\Delta t}$ cross over the boundary in a time step, Δt, and each one transports an equivalent of a "normal, diffusive, phase-space speed" of value $\sqrt{B^{(n)(n)}/\Delta t}$. In this example, $[B^{(n)(n)}P^+]^S = 0$ simply implies an overall zero value of the product of the number of particles crossing S because of diffusion times its "normal, diffusive, phase-space speed"; that is to say, if an equivalence of linear momentum in phase space were defined, its diffusive contribution at each point of S would be zero when all contributions coming from all senses were computed. Two different physical pictures, in a particle method, may be applied to explain the previous behaviour: either as many particles as those lost because of diffusion from G into G_1, weighted by $B_G^{(n)(n)}$, are replaced by particles coming by diffusion from G_1 into G, weighted by $B_{G1}^{(n)(n)}$, or particles that should cross S because of diffusion are reflected at S and return into their original domain. In both pictures, the value of $(B^{(n)(n)}P^+)_G$ coming in must be the same as that going out. $(B^{(n)(n)}P^+)_G = (B^{(n)(n)}P^+)_{G1}$ is straightforwardly imposed with the reflection picture; as long as, with a picture based on the existence of a diffusive exchange between G and G_1, it is necessary to recompute the value of $B^{(n)(n)}$ for each particle crossing S and modify the number of particles crossing ($B^{(n)(n)}P^+$ preserved).

Care has to be taken to distinguish between bulk diffusion and gradient diffusion: the probability current, Φ^n, comprises a contribution due to the gradient of $B^{(n)(n)}P^+$ which must be interpreted in terms of either absorption/emission or transmission since it is, technically, an extra drift contribution; on the other hand, the bulk value of $B^{(n)(n)}P^+$, its exact value at the boundary, is related to reflection. In practical problems, it might be difficult to extrapolate the exact value of $B^{(n)(n)}P^+$ at the boundary, from inner values, since the presence of a stiff gradient in its functional dependence close to the boundary is not excluded. Some information about the intensity of reflection and its possible random delay with an exponential dependence on time (sticky boundary condition [12]) is needed to accurately describe boundary conditions.

Renormalization has a very natural physical interpretation [21]: the global probability in $\mathbb{R}^M = G \cup S \cup G_1$ is preserved since its boundaries are at ∞ and cannot be reached, but this is not necessarily true when speaking of the probability restricted to $\overline{G} = G \cup S$. According to this interpretation P^+ is really the probability conditioned to $z \in G$ and P_S is really the probability conditioned to $z \in S$ and exchanges with G_1 (the probability conditioned to $z \in G_1$) are not excluded. The renormalization implies that the partial weight of the integration of the global PDF in the region where it is conditioned, is used as a divisor of the conditioned PDF.

The overall picture of the derivation presented in this paper is that of a weak formulation similar to that employed in generalised function analysis [22] to develop derivatives in a generalised sense

$$\frac{\partial f}{\partial z^j} = \left\{\frac{\partial f}{\partial z^j}\right\} + [f]^S \cos(\boldsymbol{n}\cdot z^j)\delta_S$$

$$\frac{\partial^2 f}{\partial z^i \partial z^j} = \left\{\frac{\partial^2 f}{\partial z^i \partial z^j}\right\} + \frac{\partial}{\partial z^i}([f]^S \cos(\boldsymbol{n}\cdot z^j)\delta_S) + \left[\left\{\frac{\partial f}{\partial z^j}\right\}\right]^S \cos(\boldsymbol{n}\cdot z^i)\delta_S$$

where f is a functional defined by a class C^2 function, $G \cup G_1 \to \mathbb{R}$, with a possible discontinuity in both its value and its derivatives at S, which acts on a space of test functions through an integration with the differential form dV. Partial derivatives to the left of the previous expressions mean derivatives in the generalised function sense whereas partial derivatives between the symbol {} mean derivatives in the standard function sense.

Looking at either (22) or (24), a weak interpretation may be given to the origin of Ito calculus or of the formula to relate drift coefficients in Chapman-Kolmogorov differential equations and in SDE according to Stratonovich. In a weak sense, a Taylor series expansion up to second order is needed to compute time evolutions to first order in time since the underlying stochastic processes show a first order in time contribution coming from the second order of the Taylor series. The problem is now that the second order term of the Taylor series is not a scalar field since it is the contraction of a second-order contravariant tensor, the diffusion one, with a second-order partial derivative of a scalar test function which is not a second-order tensor (though the first-order partial derivative is indeed a covector). The need that all laws of physics be written in a manifest covariant form leads in a natural way to either Ito calculus for the transformation of drift terms or Stratonovich relation between drift in a SDE and the equivalent Chapman-Kolmogorov differential equation. The lack of manifest covariance in the second-order term (in Taylor sense, first-order in time) only may be compensated with the corresponding modification in the first-order term (in Taylor and time sense) which stops being manifest covariant so that the addition of both terms preserves manifest covariance.

5 Comparison with Previous Work

Master and birth-death terms do not pose new problems because of the presence of a singularity at the boundary, in comparison to the situation without it. These terms were included by the sake of completeness and their analysis follows the standard situation [9] without singularities provided that care is taken to isolate regular from singular zones when computing them. Of course, were this terms present at the boundary, the overall balance of drift-diffusion contributions should match that of master-birth-death ones.

5.1 One Dimensional Case

In the one dimensional case, the boundary reduces to a discrete set of points which establish the intervals in $\mathbb{R}$ where the probability is defined. The case with two extremal points defining a single interval is the simplest one and the addition of more intervals does not pose any technical problem apart from the need of master processes to account for the exchange of probability among them if such exchanges occur. Feller [7, 8] studied thoroughly this problem under the following assumptions: the metrics in $\mathbb{R}$ is Euclidean ($g^{1/2}=1$), there are neither moving boundaries, nor birth-death processes, nor inner jumps in the regular zone, nor direct jumps from the inner zone into the extremal points; however jumps between extremal points and from them into the inner regular zone are considered, and, finally, no probability flow from or into G_1 is allowed. Under the previous assumptions, the set of PDF equations reduces to

$$\frac{\partial P^+}{\partial t} = -\frac{\partial AP^+}{\partial z} + \frac{1}{2}\frac{\partial^2 BP^+}{\partial^2 z} + W(z|r1;t)P_S(r1;t) + W(z|r2;t)P_S(r2;t) \tag{50}$$

$$\begin{aligned}\frac{\partial P_S(r1;t)}{\partial t} &= -\frac{1}{2}\frac{\partial BP^+}{\partial z}\Big|_{r1} + AP^+\big|_{r1} - \int W(x|r1;t)P_S(r1;t)\,dx\\ &\quad + W_S(r1|r2;t)P_S(r2;t) - W_S(r2|r1;t)P_S(r1;t)\end{aligned} \tag{51}$$

$$\begin{aligned}\frac{\partial P_S(r2;t)}{\partial t} &= -\frac{1}{2}\frac{\partial BP^+}{\partial z}\Big|_{r2} + AP^+\big|_{r2} - \int W(x|r2;t)P_S(r2;t)\,dx\\ &\quad + W_S(r2|r1;t)P_S(r1;t) - W_S(r1|r2;t)P_S(r2;t)\end{aligned} \tag{52}$$

$$[BP^+]^{r1} = [BP^+]^{r2} = 0 \tag{53}$$

where it is assumed that P^+ is defined in the interval $(r1,r2)\in\mathbb{R}$ and $P_S(r1;t)$ and $P_S(r2;t)$ represent the weight of Dirac deltas at boundary points $r1$ and $r2$. Since the boundary is represented by a discrete set of points, simple layer singularities are replaced by Dirac deltas at those points and surface integrals with surface element $dS = a^{1/2}d^{M-1}\zeta$ stop making sense as does the distinction between surface PDF and surface scalar weight, so that the ratio $a^{1/2}/g^{1/2}$ does not appear in the one-dimensional version of the exchange terms between $G=(r1,r2)$ and boundaries $r1$ or $r2$.

Equations (50), (51) and (52) may be found in Sect. 10 of [8], see also Chap. 3 of [2] with a different naming convention and arrangement of terms. As it has been said, the restriction given by (53) should not be confused with a limitation in the kind of boundary conditions that may be imposed on this problem. In effect, $[BP^+]^{ri} = \lim_{z\to ri} BP^+|^{G1} - \lim_{z\to ri} BP^+|^{G}$ means that there is an exact balance between local diffusive processes going out and coming into $(r1,r2)$ at points $\{r1,r2\}$, which is related to the presence of reflection at the boundaries, but it does not pose any limitation on the intensity of such diffusive processes. A thorough review of the appropriate boundary conditions for this problem may be found elsewhere [2, 8, 12].

5.2 Liouville's Equations

Liouville equations are characterised by the absence of diffusion. This problem has already been studied [21] under the same assumptions as those used in this paper. The derivation for the Liouville case is wide easier since the pure drift contribution has a contravariant vector nature and neither Ito nor Stratonovich rules are needed, just those of standard calculus. With these points in mind, Liouville's versions of (38), (39) and (40) were obtained; there is no Liouville's equivalent of (41) since it only contains a diffusion term; a possible need of renormalization was explicitly considered as well as the chance of having moving boundaries. It should be noticed that, in the original reference [21], no distinction was made between proper PDF's and scalar weight functions with a derivation which, implicitly, used scalar weights and that contributions from an external domain, G_1, were only considered in the absence of singularities at the boundaries.

5.3 Problems in Fluid Mechanics

As it was said in the Introduction, singularities at the boundary appear naturally in the stochastic representation of turbulent fluctuations of scalar fields in jets or mixing layers in Fluid Mechanics, with the singular boundary contribution corresponding to the outer laminar zone. Klimenko and Bilger [11, 13] arrived at the restriction $[BP^+]^S = (BP^+)_G = 0$, for this one-dimensional (in scalar concentration phase-space) problem, from purely physical arguments: conservation of probability (G_1 only consists of physically forbidden values and, thus, it is meaningless to consider any probability coming from it or going to there), constancy of the mean value of scalar field fluctuations due to turbulent mixing and time evolution of the variance of these fluctuations according to the law $d\langle c^2\rangle/dt = -2\langle\varepsilon_c\rangle$ where $2\langle\varepsilon_c\rangle$ is the scalar fluctuation dissipation rate.

More recently [17], there has been some discussion about different particle numerical methods fitted to elastic (partial reflection) regular boundary conditions in the stochastic simulation of velocities and densities of a fluid. The problem comes from the naming convention chosen in the Fluid Mechanics community to talk about inflow and outflow boundaries, based on physical considerations related to the mean flow behaviour, drift in the stochastic model. This led, in some instances, to neglect back-scatter, reflection induced effects typical of mathematical regular boundary conditions, with a physical correlate in the real fluctuations of the physical flow. It is worth noting that there are numerical methods following both the reflection picture [17] and the flow from the outside (particle buffer layers around the boundaries) one [23].

5.4 Fast Diffusion Layer

The study of fast diffusion layers [16] led to a derivation of Fokker-Planck equations from Chapman-Kolmogorov ones, similar to that proposed in this paper. The main differences arise from the more formal character of the present paper; here all terms are retained in the derivation without assuming that they should be zero based on particular physical considerations. In this paper, moving boundaries are considered. The conditions needed for the application of the divergence theorem by means of manifest covariant combinations of non-covariant terms have been carefully analysed. No assumption about the boundary values of test functions and their derivatives has been made in this paper. Possible contributions from an outer probability reservoir in G_1 have been considered, leading, on the one hand to the need of a renormalization of the computed PDF when these contributions are related to probability currents with a global non-zero weight and, on the other hand, to a consideration of terms with derivatives of test functions as a way of representing reflection at the boundary instead of neglecting them by the assignment of a value to the derivative of allowed test functions. Anyway, boundary conditions as established in (88) of [16] may be compared with the results of this paper. That comparison will be realized with scalar weight results, since surface integrals over the form dS are used in the reference to check with. It should also be noticed that the normal to S has opposite sense in that reference and that there is no $1/2$ factor in the diffusion terms.

Some comments on the physical assumptions used in modelling a fast diffusion layer: no jumps and birth processes are considered; there is a death process at the boundary representing the trapping of some particles in it; there are no inertial contributions at the boundary; there are no boundary singularities, though transport coefficients show singular behaviour at the boundary which is a fast diffusion layer; there is no interaction with the external medium what leads to enforcing values of the gradient of test functions at the boundary in the original reference; nevertheless, environment, according to the analysis in Sect. 4, coefficients affected by normal gradients of test functions could be isolated and related to reflection which, in turn, may be linked to the presence of a external environment supplying as much probability as that lost by bulk diffusion at the boundary.

Under the previous assumptions, the starting point of the analysis from the point of view of this paper would be

$$\begin{aligned}
&\frac{\partial \overline{P^+}}{\partial t} = -\overline{\Phi}^{i}_{;i} \quad \text{Fokker-Planck in the inner domain}\\
&\overline{\Phi}^{n}_{G} - \frac{1}{2}(B^{\alpha n}\overline{P^+})_{G;\alpha} = 0 \quad \text{probability currents at the boundary}\\
&(B^{(n)(n)}\overline{P^+})_{G1} - (B^{(n)(n)}\overline{P^+})_{G} = 0 \quad \text{reflection}
\end{aligned}$$

and the fast diffusion layer is represented, based on physical assumptions, by

$$(1/2)(B^{\alpha n}\overline{P^+})_{G;\alpha} = \sigma\overline{P^+}_G + \overline{\Phi}^{\alpha}_{G;\alpha} \tag{54}$$

where $\overline{\Phi}^{\alpha}_{;\alpha}$ represents a fast forward Fokker-Planck transport restricted to S. The death term restricted to S could also be interpreted as a probability current going into G_1 and disappearing from the integration domain. An expression equivalent to (88) of [16] would read, with the naming conventions of this paper, as

$$-\left[\overline{\Phi}^{n}\right]^{S} = -\sigma\overline{P^+}_{G1} + \overline{\Phi}^{n}_{G} = \overline{\Phi}^{\alpha}_{G;\alpha} \tag{55}$$

where it has been assumed that $\overline{P^+}$ has been continuously extended into G_1, $\overline{P^+}_{G1} = \overline{P^+}_G$, and it should be remembered that the normal to S points into opposite senses in this paper and the expression to check with.

The derivation of the boundary condition $(1/2)(B^{\alpha n}\overline{P^+})_{G;\alpha} = \sigma\overline{P^+}_G + \overline{\Phi}^{\alpha}_{;\alpha}$ deserves more attention. It results from isolating a small layer adjacent to S from the rest of the domain. Its thickness is proportional to $\sqrt{\tau}$, with τ being a small time characteristic of random walks in the inner domain. The contribution from this layer would give all the boundary singular terms under the limit $\tau \to 0$; on the other hand, the contribution from the divergence theorem applied to the rest of the domain would yield the exchange terms between the singularity and the inner domain, under the same limit.

The first physical assumption is that the small layer and the inner domain are effectively decoupled, that is to say, contributions coming from each of these terms must vanish separately, while their joint cancellation has been assumed throughout this paper. This assumption may be based on the fact that the characteristic time scale of random walks inside the small limiting layer is $\tau_a \ll \tau$ (fast diffusion layer), so that the exchange contribution to compensate with the narrow layer one, for times $\tau_a \ll t \ll \tau$, is frozen from the viewpoint of the small layer. Moreover, under the limit $\tau \to 0$, this frozen contribution becomes zero. When τ is small but not zero, it could be argued that the behaviour of the separate balance of the exchange terms is the same as in the limiting case and so is the separate balance of the small layer contribution, though this is only an assumption.

From the fact that $\tau_a \ll \tau$, an analysis of the small layer contributions may be performed [16] where it is found that terms not tending to zero in the limit $\tau_a \to 0$ are only those related to death in the layer, drift and diffusive transport parallel to the boundary and an extra drift normal to the layer which comes from the diffusion normal to the layer with time scale τ. This analysis is valid regardless of the presence or absence of a singularity at the boundary and would mean that, in (44), $\overline{A}_S^n \gamma_S - (B_S^{n\alpha}/2)\gamma_{S;\alpha} = -\overline{\Phi}_S^n = 0$ and $(B_S^{n\alpha}\gamma_S/2)_{;\alpha}$ should be moved to (43) whereas $B^{(n)(n)}\gamma_S/2$ should be moved from (45) (which would disappear) to (44). The reason being that diffusion normal to the boundary is replaced by equivalent drift terms normal to the layer what, in a formal mathematical sense, is tantamount to reducing the order of the normal derivatives of test functions linked to the corresponding terms. From this analysis and assuming the decoupling between singular (small layer) terms and exchange (divergence of the rest of the domain) ones and that there is no singular inertial contribution, (43) would become

$$-\overline{\Phi}_{S;\alpha}^{\alpha} + (B_S^{n\alpha}\gamma_S/2)_{;\alpha} - \mathfrak{D}_S\gamma_S = 0 \tag{56}$$

where $\mathfrak{D}_S = \sigma$ is the rate of trapping of particles being in the small layer. $(B_S^{n\alpha}\gamma_S/2)_{;\alpha}$ has changed sign since it comes from a volume integral of a test function times the double layer singularity with weight $(B_S^{n\alpha}\gamma_S/2)_{;\alpha}$, which is equal to a surface integral of this weight with opposite sign times the normal derivative of the test function and, after moving terms, normal derivatives of test functions become test functions.

The second physical assumption is that, in the limit $\tau \to 0$, the behaviour of $(B^{n\alpha}\overline{P^+}/2)_{G;\alpha}$ is like that of its singular counterpart as given by (56), that is to say (54) is true. It could be argued to the contrary that, in the first assumption, singular and exchange terms were assumed to be decoupled and, now, it is said that there is a exchange contribution like their singular counterpart. Both ideas may be reconciled only in the limit $\tau \to 0$.

6 Conclusions

A proper manifest covariant derivation of the Chapman-Kolmogorov differential equations with an explicit computation of surface terms, which may contain singular boundary contributions, has been presented. Work has been performed with PDF's and with related scalar weight functions [20] since the PDF does not behave as an scalar under a coordinate transformation.

Not surprisingly, this weak derivation looks like the results obtained for generalised function derivatives with explicit consideration of discontinuities at boundaries. The calculation of the inertial term could be considered as a valid generalised function derivative with regard to a standard variable (time), instead of a generalised one (stochastic phase space) when the domain in the generalised phase space depends on the value of the standard variable (moving boundaries).

The drift, as usually considered in Fokker-Planck equations, is not a contravariant vector. Graham [10] proposed a modified, contravariant drift $A^i - (1/2g^{1/2})\partial(B^{ij}g^{1/2})/\partial z^j$ (g is the determinant of the covariant metrics) which leads straightforwardly to the Stratonovich form of Chapman-Kolmogorov differential equations with singular terms at the boundary. In this paper, a different modification has been identified: $A^i + \Gamma^i_{kl}B^{kl}$. This version does not modify the drift when the metrics connection is zero, such as it is the case with Cartesian coordinates in an Euclidean metrics and with a connection compatible with the metrics. It leads straightforwardly to the standard form of Chapman-Kolmogorov differential equations with singular terms at the boundary. Of course, both modified drifts and both forms of Fokker-Planck equations are related.

The rules of Ito and Stratonovich stochastic calculus may be interpreted in a weak sense as a way of preserving manifest covariance when second order terms in a Taylor series expansion of test functions have to be retained together with first order terms.

A physical picture of singular boundary contributions has been provided in terms of Monte Carlo particles with their expected interaction with a boundary: absorption, emission, transmission and reflection.

A comparison with previous work on the topic has been conducted.

Some points to bear into mind since their modification would imply a change in the results of this paper are:

(i) The limit for short times of the ratio between higher order statistical moments of small displacements and Δt, in the form of (6) and (7), vanish with the maximum displacement considered. That is to say, work is done with Markov processes and a well-defined PDF [9] (positive semi-definite and normalizable).

(ii) The domain metrics is assumed to be continuous in $\mathbb{R}^M$ and constant in time. Were g to depend on time, there would be additional inertial terms like that displaying time evolution of a in (8) plus an advection-like term which was excluded from the evolution of a because it was considered that S, as an $M-1$ manifold embedded in $\mathbb{R}^M$, propagates normal to itself.

(iii) There is not a chain of singularities inside singularities in manifolds with a dimension progressively reduced. It has not been considered that there was an $M-2$ manifold embedded in S such that the values of P_S, γ_S, A^α_S or $B^{\alpha\beta}_S$ showed any discontinuity at it. If so, S could be divided into regular zones (regular from intrinsic consideration, not from M space view) separated by $M-2$ manifolds playing the role of boundaries inside S and the application of the divergence theorem to each bounded zone inside S would stop giving a zero contribution; that is to say, singularities (from the intrinsic view of S) could develop at those $M-2$ manifolds. The chain of singularities inside singularities could be continued until arriving at singular points.

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