

# A systematic path to non-Markovian dynamics II: Probabilistic response of nonlinear multidimensional systems to Gaussian colored noise excitation

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**Abstract:** The probabilistic characterization of non-Markovian responses to nonlinear dynamical systems under colored excitation is an important issue, arising in many applications. Extending the Fokker-Planck-Kolmogorov equation, governing the first-order response probability density function (pdf), to this case is a complicated task calling for special treatment. In this work, a new pdf-evolution equation is derived for the response of nonlinear dynamical systems under additive colored Gaussian noise. The derivation is based on the Stochastic Liouville equation (SLE), transformed, by means of an extended version of the Novikov-Furutsu theorem, to an exact yet non-closed equation, involving averages over the history of the functional derivatives of the non-Markovian response with respect to the excitation. The latter are calculated exactly by means of the state-transition matrix of variational, time-varying systems. Subsequently, an approximation scheme is implemented, relying on a decomposition of the state-transition matrix in its instantaneous mean value and its fluctuation around it. By a current-time approximation to the latter, we obtain our final equation, in which the effect of the instantaneous mean value of the response is maintained, rendering it nonlinear and non-local in time. Numerical results for the response pdf are provided for a bistable Duffing oscillator, under Gaussian excitation. The pdfs obtained from the solution of the novel equation and a simpler small correlation time (SCT) pdf-evolution equation are compared to Monte Carlo (MC) simulations. The novel equation outperforms the SCT equation as the excitation correlation time increases, keeping good agreement with the MC simulations.

**Keywords:** random differential equations; generalized Fokker-Planck-Kolmogorov equations; stochastic dynamical systems; response pdf-evolution equation; colored noise excitation; nonlinear stochastic processes;

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## 1. Introduction

Stochastic modeling of dynamical systems, initiated in the first decade of the 20<sup>th</sup> century in statistical physics [1, 2] and finance [3, 4], has been constantly expanding, establishing a strong presence in science and engineering. In the 21<sup>st</sup> century, stochastic modeling flourished further and infiltrated almost any mathematics-based discipling, from theoretical physics and engineering sciences to biology, climate, economics and more.

In view of this vast landscape, we restrict ourselves to the area of macroscopic stochastic dynamics, for which a mathematical prototype is a system of nonlinear differential equations under random excitation. Such a system will be abbreviated subsequently as RDE (Random Differential Equations) [Abbreviations are defined in first appearance. For reader's convenience, an alphabetical list of abbreviations is given as Appendix A]. The random excitation may be Gaussian or non-Gaussian, delta-correlated or smoothly-correlated, and may appear in the RDE either additively or multiplicatively. All three dichotomies mentioned above are important, and any specific combination of them leads to specific difficulties and peculiarities. The dichotomy between delta-correlated and smoothly-correlated excitation, which is the main concern of the present paper, has profound implications on the probabilistic characterization of the response, and on the theoretical and methodological background needed for treating the RDE.

The case of delta-correlated stochastic excitation (white noises) is the most intensively studied case in the current literature. In this case, it is well known that the response is Markovian, and the complete description of response's probabilistic structure is given by the transition pdf, governed by the Fokker-Plank-Kolmogorov equation (FPKE) [5, 6], [7] Sec. 5.6.6,[8] Ch. 5, [9] Sec. 6.3, or by the Kolmogorov-Feller equation [10–12].

However, “*the nature knows no delta-correlated processes. All actual processes and fields are characterized by a finite temporal correlation radius, and delta-correlated processes and fields result from asymptotic expansions in terms of their temporal correlation radii*” Klyatskin (2005) [13], p. 91. Even though smoothly-correlated (colored) excitation is a more realistic model, better suited to the mathematical modeling of stochastic dynamics problems, remains poorly studied up to now, probably due to its increased difficulty. By assuming colored excitation, the response loses its Markovian character, and its probabilistic structure cannot be inferred by a single probability density function (pdf). In that case, the complete probabilistic description of the response requires the determination of the infinite hierarchy of pdfs of various orders (one-time, two-times etc.), rendering the problem unsolvable in the current state-of-the-art. The alternative formulation, using the characteristic functional and the Hopf's equation (see [14], Introduction, for a discussion and references), is promising but also remains beyond the capabilities of the present research state; see e.g. [15], Sec. 2.1.5. A modest, feasible alternative is to formulate approximate equations, separately for each order. Such kind of equations for the first-order (one-time) pdf have been developed in some cases, and are usually termed *generalized FPKE* (genFPKE). Their formulation is a difficult task since, in the non-Markovian case, all orders of pdfs are coupled and thus, an efficient, approximate decoupling technique is required. In this paper, a systematic approach is developed for deriving genFPKE for the first-order, response pdf, corresponding to multidimensional, nonlinear, dynamical systems under additive Gaussian excitation. Needless to say, the scalar problem has been much more extensively studied [16–24]. An extensive review of methods

for constructing genFPKE for this case can be found in [14, 25]. The present work is a sequel of [25], generalizing its methodology to the multidimensional case. The literature survey presented below mainly refers to the multidimensional problem, on which the present work is focused.

### 1.1 *Literature survey*

The importance of exploiting the colored noise excitation has been well appreciated in applications [26–31]; besides, the complications that emerge from this modeling have been already pointed out [14, 22, 25, 29, 32–35] [36] Sec IX.7. To this end, various approaches have been developed through time, shaping the methodological inventory for non-Markovian responses. First, and probably most known among engineering audience, is the filtering approach [7], Sec 5.10, [22, 37], also called Markovianization method [38], in which the RDE system is augmented by linear filters fed by white noises and producing as output an approximation of the colored excitation. This approach allows the formulation of a FPKE (for the augmented system, including the filters), avoiding uncharted waters. However, the increment of the degrees of freedom, due to the presence of the filters, leads to an undesirable inflation of the spatial dimensions of the final FPKE.

Alternative lines of work, based on more fundamental considerations, initiated in the works of Lax [39], Van Kampen [40], Fox [41], and Hanggi [42]. Derivations of genFPKE corresponding to multidimensional RDE, usually under the assumption of Gaussian excitation, have been mainly developed by means of two generic methodologies: the *functional calculus approach* [33, 43–45], and the *cumulant expansion approach* [46, 47]. In both approaches the starting point is the Stochastic Liouville Equation (SLE) corresponding to the RDE. The SLE is exact, yet non-closed, and further considerations are required for the derivation of an approximate, solvable, genFPKE. The latter is more complicated than the standard FPKE obtained by Markovianization, but its spatial dimension coincides with the state-space dimension of the underlying system of RDE.

In the functional calculus approach, the Novikov-Furutsu (NF) theorem [48, 49] is usually invoked to implement correlation splitting between response and excitation. The resulting equation contains the Volterra functional derivative of the response with respect to the excitation [34, 40, 50], conveying non-local features in the formulation. The treatment of the Volterra derivative is crucial and has been addressed by two methods. The *correlation time expansion method* [44, 45], based on the small correlation time (SCT) assumption, utilizes an asymptotic expansion of the derivative around the current time, deriving approximate genFPKE, hierarchized by the correlation time orders. Alternatively, the Volterra derivative has been *explicitly calculated* without assuming SCT approximation [33, 43], resulting in a non-closed master equation [43], which requires a closure argument to become solvable [42].

In the cumulant expansion method the NF theorem is not utilized. Instead, the SLE is transformed into the interaction picture [51], [52], Ch. 7, allowing the excitation's generalized cumulants to be employed [53] Sec. II.1, [54–57]. The resulting master equation is exact but non-closed, containing an infinite superposition of ordered cumulants. Under the assumption of weakly correlated excitation, the equation can be truncated at a specific order, and using a current time approximation, genFPKE corresponding to each order can be formulated. Results obtained by Fox [47] using the cumulant expansion method, coincide with Dekker's

[44] using the correlation expansion method. Further, the cumulant expansion method has also been applied to Poisson noise [58].

Two more methods for constructing genFPKE, mainly implemented for the scalar case, are the *projection operator method* [59–63] and the *unified colored noise approximation* (UCNA) [64], [22] Sec. V.C. Extensions of these methods to the multidimensional case have recently been published; see [65], [66].

## 1.2 *Structure of the present work*

In the present work we derive and validate new pdf-evolution equations (a novel genFPKE) governing the pdf dynamics of the response vector of a system of nonlinear and non-autonomous RDEs, under additive Gaussian excitation. In Section 2, we first formulate the underlying dynamical problem and the corresponding SLE. Then, we briefly describe the methodology used for the derivation of the new genFPKE and summarize the main results of this work. The detailed exposition of the derivation starts in Section 3, where we utilize an extended form of the NF theorem [49] to obtain a novel version of the SLE, called herein *transformed SLE*, which is exact but non-closed. In Section 4, we present some simple applications of the transformed SLE. We consider three simple problems: *linear* systems of RDEs under general Gaussian excitation, nonlinear systems of RDEs under white noise excitation, and nonlinear systems of RDEs under colored noise excitation of small correlation time. In the first two cases the closure is automatic. Especially in the second problem we (re)derive the classical FPKE in a simple and straightforward way. In the third problem we derive a SCT approximate genFPKE, again in a surprisingly easy and straightforward manner, which does not seem to have been given explicitly in the literature. The main original contribution of this paper is presented in Section 5, where a new closure technique is applied to the transformed SLE, permitting us to derive a novel pdf-evolution equation which outperforms the SCT model. In Section 6, first numerical results are presented for a bistable Duffing oscillator. The obtained response pdf, both in the transient and the steady-state regime, are nicely compared with results obtained by using Monte Carlo simulation. Finally, in Section 7, we provide a critical discussion of the methodology and the findings of this work, as well as ideas for improving the pdf-evolution equation and extending it to more general problems.

## 2. Formulation of the problem and main results

### 2.1 *Formulation of the problem and preliminary discussion*

The problem we are dealing with in this paper is the determination of the one-time probabilistic structure of the response of an  $N$  – dimensional, nonlinear system of RDEs, under generic colored Gaussian additive excitation. The system of RDEs can be written in the form

$$\dot{X}_n(t; \theta) = h_n(\mathbf{X}(t; \theta), t) + \Xi_n(t; \theta), \quad (2.1a)$$

$$X_n(t_0; \theta) = X_n^0(\theta), \quad n = 1, 2, \dots, N, \quad (2.1b)$$

where the overdot denotes differentiation with respect to the time  $t$ ,  $\theta$  denotes the stochastic argument, and the deterministic functions  $h_n(\mathbf{x}, t)$  are assumed to be Lipschitz continuous in  $\mathbf{x}$  and continuous in  $t$ . The random excitations  $\Xi_n(t, \theta)$  and the random initial values

$X_n^0(\theta)$  are the *data of the system*, and thus they are assumed to be known. We shall follow the usual (useful and convenient) assumption that the random data are Gaussian. More precisely, the vector  $\mathbf{X}^0(\theta) = \left( X_n^0(\theta) \right)_{n=1}^N$  and the vector function  $\Xi(t, \theta) = \left( \Xi_n(t, \theta) \right)_{n=1}^N$  are considered *jointly Gaussian*. Their probabilistic structure is completely defined by means of their mean vectors  $\mathbf{m}_{X^0}$  and  $\mathbf{m}_{\Xi(\cdot)}(t)$ , the autocovariance matrices  $\mathbf{C}_{X^0 X^0}$ ,  $\mathbf{C}_{\Xi(\cdot)\Xi(\cdot)}$ , and the cross-covariance matrix  $\mathbf{C}_{X^0 \Xi(\cdot)}$ . Let it be noted that, to the best of our knowledge, the case where excitations are correlated to the initial values have not been studied before, with the exception of papers [18, 34, 49], dealing with the scalar problem, by the present research group.

The starting point of the probabilistic study of systems (2.1a) is the representation of the response pdf as an *averaged random delta function* [17–19, 21, 43, 44, 67–69], also called *pdf method* in the theory of turbulence [70, 71] or *delta projection method* in [25, 34]. Employing the notation  $f_{X(t)}(\mathbf{x}) = f_{X_1(t) X_2(t) \dots X_N(t)}(x_1, x_2, \dots, x_N)$  for the *one-time response pdf*, the delta projection method is based on the representation:

$$f_{X(t)}(\mathbf{x}) = \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \right], \quad (2.2)$$

where

$$\delta(\mathbf{x} - \mathbf{X}(t; \theta)) = \delta(x_1 - X_1(t; \theta)) \times \dots \times \delta(x_N - X_N(t; \theta)), \quad (2.3)$$

is a *multidimensional random delta function*. By differentiating both sides of equation (2.3) with respect to time, employing the identity

$$\frac{\partial \delta(\mathbf{x} - \mathbf{X}(t; \theta))}{\partial t} = - \frac{\partial \delta(\mathbf{x} - \mathbf{X}(t; \theta))}{\partial \mathbf{x}} \cdot \dot{\mathbf{X}}(t; \theta),$$

or, equivalently,

$$\frac{\partial \delta(\mathbf{x} - \mathbf{X}(t; \theta))}{\partial t} = - \sum_{n=1}^N \dot{X}_n(t; \theta) \delta'(x_n - X_n(t; \theta)) \prod_{\substack{j=1 \\ j \neq n}}^N \delta(x_j - X_j(t; \theta)),$$

and substituting the resulting time derivative of the response vector by using equation (2.1a), we obtain the corresponding *Stochastic Liouville equation* (SLE), after averaging:

$$\begin{aligned} \partial_t f_{X(t)}(\mathbf{x}) + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left( h_n(\mathbf{x}, t) f_{X(t)}(\mathbf{x}) \right) &= \\ &= - \sum_{n=1}^N \frac{\partial}{\partial x_n} \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \Xi_n(t; \theta) \right]. \end{aligned} \quad (2.4)$$

Note that, in equation (2.4), the ensemble average  $\mathbb{E}^\theta[\cdot]$  should be taken with respect to the joint response-excitation probability measure  $P_{X(\cdot)\Xi(\cdot)}$ . If the external excitation is zero,

$\Xi(t; \theta) = 0$ , the above equation is reduced to the classical *Liouville-Gibbs equation* [72]. The terminology *Stochastic Liouville equation* was introduced by Kubo in 1963 [73]. Even though equation (2.4) is exact, deterministic, and its left-hand side has the form of a first order PDE with respect to  $f_{X(t)}(\mathbf{x})$ , the averages:

$$\begin{aligned} \mathcal{N}_n^{X\Xi}(\mathbf{x}, t) &\equiv \mathcal{N}_n^{X\Xi} := \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \Xi_n(t; \theta) \right] = \\ &= \int_{\mathbb{R}} \xi_n f_{X(t)\Xi_n(t)}(\mathbf{x}, \xi_n) d\xi_n, \quad n = 1, \dots, N, \end{aligned} \quad (2.5)$$

in the right-hand side, involve the joint response-excitation pdfs  $f_{X(t)\Xi_n(t)}(\mathbf{x}, \xi_n)$ , making the equation non-closed. Aiming to derive a closed evolution equation for  $f_{X(t)}(\mathbf{x})$ , we employ the extended (multidimensional) Novikov-Furutsu (NF) Theorem [34, 49], to eliminate the dependence of  $\mathcal{N}_n^{X\Xi}$  on the corresponding stochastic excitation. An important implication of this procedure is that the terms  $\mathcal{N}_n^{X\Xi}$  become non-local in time.

Starting with equation (2.4), in Section 3, we reformulate it by using the extended NF Theorem [49], obtaining a transformed SLE which contains averages over the derivatives of  $\mathbf{X}(t; \theta)$  with respect to the initial values  $X_n^0(\theta)$  and the excitation functions  $\Xi_n(s; \theta)$ ,  $s < t$ , called herein *variational derivatives*. The second ones are Volterra functional derivatives [74], [2]. These derivatives contain the unknown response, satisfying linear, time-varying ODEs (Ordinary Differential Equations), namely, the *variational problems* associated with equations (2.1a,b). The treatment of these terms is critical for deriving a “good” pdf-evolution equation. In contrast to all other approaches, in this paper we solved the variational problems exactly, in terms of the state-transition matrices. The latter contains the time history of response function  $\mathbf{X}(t; \theta)$ , retaining the non-local and non-closed character of the equation. Nevertheless, the exact character of solutions for the variational derivatives permits us to perform a highly improved treatment of the corresponding terms, leading to efficient, approximate pdf-evolution equations. The main steps towards obtaining improved closed equations are the separation of the (instantaneous) mean value of the response from its random fluctuations, and the use of the Magnus expansion to obtain handy, explicit formulae for the state transition matrices. This permits us to keep intact and treat exactly the effect of the instantaneous mean values of the response (modeled as time-integrals of some generalized response moments), restricting the eventual current time approximation to the random fluctuations only. To the best of our knowledge, this treatment is innovative and applied for the first time to this kind of problem. It leads to new closed, nonlinear, and non-local pdf-evolution equations, significantly improved in comparison of those based on the SCT approximation schemes. Our equations share features with mean-field nonlinear FPKE, as presented by [75], but it also exhibits non-locality in time, a feature reflecting the non-Markovian character of the response. The form of these equations is presented in the next subsection, along with a brief comparison with the classical FPKE.

## 2.2 Main results: A new, closed, solvable pdf- evolution equation for non-Markovian response

The main result of the present paper, being derived in Section 5, is the following pdf-evolution equation, governing the one-time response pdf of the nonlinear system (2.1):

$$\begin{aligned} \frac{\partial f_{\mathbf{x}(t)}(\mathbf{x})}{\partial t} + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left[ \left( h_n(\mathbf{x}, t) + \underline{m_{\Xi_n(\cdot)}(t)} \right) f_{\mathbf{x}(t)}(\mathbf{x}) \right] = \\ = \sum_{n=1}^N \sum_{\nu=1}^N \frac{\partial}{\partial x_n} \frac{\partial}{\partial x_\nu} \left[ \left( \underline{\mathcal{D}_{\nu n}^{X_0 \Xi(\cdot)}} [f_{\mathbf{x}(\cdot)}(\cdot); \mathbf{x}, t] + \underline{\underline{\mathcal{D}_{\nu n}^{\Xi(\cdot) \Xi(\cdot)}} [f_{\mathbf{x}(\cdot)}(\cdot); \mathbf{x}, t]} \right) f_{\mathbf{x}(t)}(\mathbf{x}) \right]. \end{aligned} \quad (2.6)$$

This equation exhibits both similarities and differences with respect to the classical FPKE. The simply underlined terms model the effects of the (non-zero) mean value of the excitation ( $\underline{m_{\Xi_n(\cdot)}}$ ) and of the (possible) dependance of the initial values with the excitation ( $\underline{\mathcal{D}_{\nu n}^{X_0 \Xi(\cdot)}}$ ), which usually do not appear in such kind of equations. Nevertheless, these features are not the main source of novelty of the equation (2.6). Neglecting these two terms, we see an equation structurally similar to the classical FPKE. However, this similarity with FPKE is only *apparent*. The most profound difference of equation (2.6) from FPKE (and other similar ones) lies within the doubly underlined diffusion coefficients  $\underline{\underline{\mathcal{D}_{\nu n}^{\Xi(\cdot) \Xi(\cdot)}}}$ . The latter are not simply functions of the state vector  $\mathbf{x}$  and the current time  $t$  (as usually), but they are, in addition, *dependent on the time history of some response moments*, namely

$$R_{ij}(t) \equiv R_{ij} [f_{\mathbf{x}(t)}(\cdot), t] = \int_{\mathbb{R}^N} \frac{\partial h_i(\mathbf{x}, t)}{\partial x_j} f_{\mathbf{x}(t)}(\mathbf{x}) d\mathbf{x}. \quad (2.7)$$

The diffusion coefficient matrix has the form

$$\underline{\underline{\mathcal{D}^{\Xi(\cdot) \Xi(\cdot)}} [f_{\mathbf{x}(\cdot)}(\cdot); \mathbf{x}, t]} = \int_{t_0}^t \mathbf{K}(\mathbf{x}, t, s) \Phi[\mathbf{R}](t, s) \mathbf{C}_{\Xi(\cdot), \Xi(\cdot)}(t, s) ds, \quad (2.8)$$

where  $\mathbf{K}(\mathbf{x}, t, s)$  is an exponential matrix, dependent on the approximation scheme, and  $\Phi[\mathbf{R}](t, s)$  is a state-transition, matrix solving the time-dependent matrix differential equation  $\dot{\mathbf{Y}}(t) = \mathbf{R}(t) \mathbf{Y}(t)$ ,  $\mathbf{Y}(s) = \mathbf{I}$ . The components of matrix  $\mathbf{R}$  are given by equation (2.7).

Equations (2.7) and (2.8) explain the nonlocal and nonlinear character of equation (2.6), which makes it essentially different from any other existing model equations for the same problem. These features are the overhead for taking into account the correlation time of the excitation and the implied non-Markovian character of the response. Nevertheless, they reward us with an equation richer than other existing ones (recovering them after simplifications), having larger range of validity with respect to the correlation time. The last statement has been confirmed by numerical results, validated by Monte Carlo simulations.

**Remark 1.** The somewhat unusual notation  $f_{X(\cdot)}(\cdot)$  used in the diffusion coefficients, expresses the fact that the corresponding dependence on the pdf  $f_{X(t)}(\mathbf{x})$  occurs by means of integration over the time history as well as over the entire state space. This becomes clear by the equations (2.7) and (2.8).

### 3. Transformation of SLE via the extended NF Theorem

#### 3.1 A second form of the SLE

According to equations (2.1a,b), the response path function  $\mathbf{X}(t; \theta)$  (for each  $\theta$ ) is uniquely determined at any specific time  $t$ , by means of the initial value  $\mathbf{X}_0(\theta)$  and the history of the excitation  $\Xi(s, \theta)$ , for all  $s \in [t_0, t]$ . To formalize and exploit this dependence, we claim that  $\mathbf{X}(t; \theta)$  is a *function-functional* (abbreviated to FF $\ell$ ) on the data  $\mathbf{X}_0(\theta)$  and  $\Xi(s, \theta)$ ,  $s \in [t_0, t]$ , and we write

$$\mathbf{X}(t; \theta) = \mathcal{X} \left[ \mathbf{X}^0(\theta); \Xi(\cdot |_{t_0}^t; \theta) \right] \equiv \left( \mathcal{X}_n \left[ \mathbf{X}^0(\theta); \Xi(\cdot |_{t_0}^t; \theta) \right] \right)_{n=1}^N. \quad (3.1)$$

That is,  $\mathcal{X}[\cdot; \cdot]$  denotes the vector function-functional representation of  $\mathbf{X}(t; \theta)$ , while  $\mathcal{X}_n[\cdot; \cdot]$  are the components of  $\mathcal{X}[\cdot; \cdot]$ , representing  $X_n(t; \theta)$ . The symbol  $\Xi(\cdot |_{t_0}^t; \theta)$  denotes the history  $\{ \Xi(s, \theta), s \in [t_0, t] \}$  of the excitation. The simpler symbol  $\Xi(\cdot; \theta)$  could, in principle, be used, but in the subsequent analysis we have to consider cases where the history of the excitation must be taken over different time intervals, e.g. the interval  $(s, t]$  or  $(s, \tau]$ , where  $t_0 \leq s < \tau \leq t$ . Thus, keeping the endpoints of the time interval in the notation, as in  $\Xi(\cdot |_{t_0}^t; \theta)$  or  $\Xi(\cdot |_{t_0}^{\tau}; \theta)$ , is a convenient way to keep track on the correct dependence in each case.

Next, we extend the FF $\ell$  point of view to the random delta function  $\delta(\mathbf{x} - \mathbf{X}(t; \theta))$ , appearing in equation (2.4), writing

$$\begin{aligned} \mathcal{F} \left[ \mathbf{X}^0(\theta); \Xi(\cdot |_{t_0}^t; \theta) \right] &= \delta \left( \mathbf{x} - \mathcal{X} \left[ \mathbf{X}^0(\theta); \Xi(\cdot |_{t_0}^t; \theta) \right] \right) = \\ &= \prod_{n=1}^N \delta \left( x_n - \mathcal{X}_n \left[ \mathbf{X}^0(\theta); \Xi(\cdot |_{t_0}^t; \theta) \right] \right). \end{aligned} \quad (3.2)$$

The symbol  $\mathcal{F}[\cdot; \cdot]$  is used to emphasize the function-functional structure of the dependence on the random data, suppressing temporarily its exact form. Using this notation, the average terms  $\mathcal{N}_n^{X\Xi}$ , equation (2.5), take the form:

$$\mathcal{N}_n^{X\Xi} = \mathbb{E}^\theta \left[ \mathcal{F} \left[ \mathbf{X}^0(\theta); \Xi(\cdot |_{t_0}^t; \theta) \right] \Xi_n(t; \theta) \right]. \quad (3.3)$$

Substituting (3.1) in the SLE (2.4), we obtain the following *second form of the SLE*, namely:

$$\begin{aligned} \partial_t f_{X(t)}(\mathbf{x}) + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left( h_n(\mathbf{x}, t) f_{X(t)}(\mathbf{x}) \right) = \\ = - \sum_{n=1}^N \frac{\partial}{\partial x_n} \left( \mathbb{E}^\theta \left[ \mathcal{F} \left[ \mathbf{X}^0(\theta); \Xi(\cdot|_{t_0}^t; \theta) \right] \Xi_n(t; \theta) \right] \right), \end{aligned} \quad (3.4)$$

Equation (3.3) (and (3.4)) reveals an interesting feature of the non-closed terms  $\mathcal{N}_n^{X\Xi}$ . They contain averages of specific (yet unknown) FF $\ell$ s of the random data, multiplied by the components of the Gaussian excitation  $\Xi_n(t; \theta)$ . This structure facilitates the application of the NF Theorem.

### 3.2 Application of the extended NF Theorem

In [34, 49] Athanassoulis and Mamis developed various extensions of the classical Novikov-Furutsu theorem [48, 76]. The one which is given (and applied) below refers to random FF $\ell$ s of the form  $\mathcal{F}[\mathbf{X}^0(\theta); \Xi(\cdot|_{t_0}^t; \theta)]$  (abbreviated as  $\mathcal{F}[\dots]$  for conciseness), whose arguments  $\mathbf{X}^0(\theta)$ ,  $\Xi(\cdot; \theta)$  are jointly Gaussian. The theorem provides the following *reduction of dependence (correlation splitting)*:

$$\begin{aligned} \mathbb{E}^\theta \left[ \mathcal{F}[\dots] \Xi_n(t; \theta) \right] = m_{\Xi_n(\cdot)}(t) \mathbb{E}^\theta \left[ \mathcal{F}[\dots] \right] + \\ + \sum_{n_1=1}^N C_{X_{n_1}^0 \Xi_n(\cdot)}(t) \mathbb{E}^\theta \left[ \frac{\partial \mathcal{F}[\dots]}{\partial X_{n_1}^0(\theta)} \right] + \\ + \sum_{n_2=1}^N \int_{t_0}^t C_{\Xi_n(\cdot) \Xi_{n_2}(\cdot)}(t, s) \mathbb{E}^\theta \left[ \frac{\delta \mathcal{F}[\dots]}{\delta \Xi_{n_2}(s; \theta)} \right] ds. \end{aligned} \quad (3.5)$$

In equation (3.5),  $\delta \cdot / \delta \Xi_{n_2}(s; \theta)$  denotes the Volterra functional derivative with respect to the excitation function  $\Xi_{n_2}(\cdot; \theta)$ , at the point (time instant)  $s$ . Setting  $m_{\Xi_n(\cdot)} = 0$  and  $C_{X_{n_1}^0 \Xi_n(\cdot)}(t, s) = 0$ , equation (3.5) reduces to the classical NF theorem [48, 76]. This classical form has been extensively used before for the formulation of genFPKE [19, 44, 45, 77–79]. The extended form of the NF theorem, equation (3.5), has been used in [25] for the study of a scalar RDE, and in [33, 34] in a preliminary analysis of the multidimensional problem.

To implement the NF theorem (3.5), we need to elaborate on the derivatives  $\partial \mathcal{F}[\dots] / \partial X_{n_1}^0(\theta)$  and  $\delta \mathcal{F}[\dots] / \delta \Xi_{n_2}(s; \theta)$ . Using equation (3.2) and keeping in mind equation (3.1), we find

$$\begin{aligned}
\frac{\partial \mathcal{F}[\dots]}{\partial X_{n_1}^0(\theta)} &= \frac{\partial}{\partial X_{n_1}^0(\theta)} \delta(\mathbf{x} - \mathbf{X}(t; \theta)) = \\
&= - \sum_{\nu=1}^N \frac{\partial \delta(x_\nu - X_\nu(t; \theta))}{\partial x_\nu} \frac{\partial X_\nu(t; \theta)}{\partial X_{n_1}^0(\theta)} \prod_{\substack{\nu_1=1 \\ \nu_1 \neq \nu}}^N \delta(x_{\nu_1} - X_{\nu_1}(t; \theta)), \tag{3.6a}
\end{aligned}$$

$$\begin{aligned}
\frac{\delta \mathcal{F}[\dots]}{\delta \Xi_{n_2}(s; \theta)} &= \frac{\delta}{\delta \Xi_{n_2}(s; \theta)} \delta(\mathbf{x} - \mathbf{X}(t; \theta)) = \\
&= - \sum_{\nu=1}^N \frac{\partial \delta(x_\nu - X_\nu(t; \theta))}{\partial x_\nu} \frac{\delta X_\nu(t; \theta)}{\delta \Xi_{n_2}(s; \theta)} \prod_{\substack{\nu_1=1 \\ \nu_1 \neq \nu}}^N \delta(x_{\nu_1} - X_{\nu_1}(t; \theta)). \tag{3.6b}
\end{aligned}$$

Note that, in equation (3.6b), we apply the chain rule for the Volterra derivative with respect to excitation  $\Xi_{n_2}(\cdot; \theta)$ . Further, we see that the essential part for the calculation of the derivatives  $\partial \mathcal{F}[\dots] / \partial X_{n_1}^0(\theta)$  and  $\delta \mathcal{F}[\dots] / \delta \Xi_{n_2}(s; \theta)$  is the calculation of the following variational derivatives:

$$V_{\nu n_1}^{X^0}(t; \theta) = \frac{\partial X_\nu(t; \theta)}{\partial X_{n_1}^0(\theta)} \equiv \frac{\partial \mathcal{X}_\nu \left[ \mathbf{X}^0(\theta); \Xi(\cdot|_{t_0}^t; \theta) \right]}{\partial X_{n_1}^0}, \tag{3.7a}$$

$$V_{\nu n_2}^{\Xi(s)}(t; \theta) = \frac{\delta X_\nu(t; \theta)}{\delta \Xi_{n_2}(s; \theta)} \equiv \frac{\delta \mathcal{X}_\nu \left[ \mathbf{X}^0(\theta); \Xi(\cdot|_{t_0}^t; \theta) \right]}{\delta \Xi_{n_2}(s; \theta)}. \tag{3.7b}$$

Derivatives (3.7a,b) express the rate of change of the response components  $X_\nu(t; \theta)$  with respect to the components of the initial values  $X_{n_1}^0(\theta)$ , and the components of the excitation  $\Xi_{n_2}(t; \theta)$ ,  $n_2 = 1, \dots, N$ , respectively. This is why they are usually called *variational derivatives* of the system (2.1) (or its solution). The variational derivatives (3.7) satisfy linear initial value problems (IVPs), formulated and solved in Section 3.3.

Using equations (3.6) and (3.7), in conjunction with the NF theorem (3.5), we readily reformulate the SLE (3.4) in the form:

$$\begin{aligned}
&\frac{\partial f_{\mathbf{X}(t)}(\mathbf{x})}{\partial t} + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left[ \left( h_n(\mathbf{x}) + m_{\Xi_n(\cdot)}(t) \right) f_{\mathbf{X}(t)}(\mathbf{x}) \right] = \\
&+ \sum_{n=1}^N \sum_{\nu=1}^N \frac{\partial}{\partial x_n} \frac{\partial}{\partial x_\nu} \sum_{n_1=1}^N C_{X_{n_1}^0 \Xi_n(\cdot)}(t) \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) V_{\nu n_1}^{X^0}(t; \theta) \right] + \\
&+ \sum_{n=1}^N \sum_{\nu=1}^N \frac{\partial}{\partial x_n} \frac{\partial}{\partial x_\nu} \sum_{n_2=1}^N \int_{t_0}^t C_{\Xi_n(\cdot) \Xi_{n_2}(\cdot)}(t, s) \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) V_{\nu n_2}^{\Xi(s)}(t; \theta) \right] ds. \tag{3.8}
\end{aligned}$$

Equation (3.8) will hereafter be referred to as the *transformed SLE*. It is exact but non-closed due to the averages over the variational derivatives, which are dependent on the whole history of excitation. Equation (3.8) is a generalization of the usually derived SLE [43–45, 80] to the case of non-zero mean excitations and excitations correlated with the initial data.

### 3.3 Calculation of the variational derivatives

The calculation of the variational derivatives will be carried out by formulating and solving the corresponding *variational problems*, obtained by differentiating the system of RDEs (2.1) with respect to the data (initial values and excitation functions). Differentiations will be carried out path-wisely, i.e., for each  $\theta$  separately. Thus, the presence of the stochastic argument  $\theta$  is not essential herein, and it is omitted in this section. We start by rewriting equations (2.1a,b) in the following form

$$\dot{X}_\nu(t) = h_\nu(\mathbf{X}(t), t) + \Xi_\nu(t), \quad (3.9a)$$

$$X_\nu(t_0) = X_\nu^0, \quad \nu = 1, 2, \dots, N. \quad (3.9b)$$

#### 3.3.1 Calculation of the variational derivatives $V_{\nu n_1}^{X^0}$

Applying the operator  $\partial \bullet / \partial X_{n_1}^0$  to both sides of the equations (3.9a,b), and recalling that each path-function  $\Xi_\nu(t)$  is not functionally dependent on  $X_{n_1}^0$ ,  $n_1 \in \{1, \dots, N\}$ , we get the following IVPs:

$$\frac{d}{dt} V_{\nu n_1}^{X^0}(t) = \sum_{v_1=1}^N \frac{\partial h_\nu(\mathbf{X}(t), t)}{\partial X_{v_1}(t)} V_{\nu v_1}^{X^0}(t) + \underbrace{\frac{\partial \Xi_\nu(t)}{\partial X_{n_1}^0}}_{=0}, \quad t_0 < t \quad (3.10a)$$

$$V_{\nu n_1}^{X^0}(t_0) = \frac{\partial X_\nu^0}{\partial X_{n_1}^0} = \delta_{\nu n_1}, \quad \nu = 1, \dots, N, \quad (3.10b)$$

where  $\delta_{\nu n_1}$  denote the Kronecker delta. Note that in equation (3.10a) we have assumed the interchangeability of derivative operators  $\partial \bullet / \partial X_{n_1}^0$  and  $d \bullet / dt$ . Under the assumption that  $\partial h_\nu(\mathbf{X}(t), t) / \partial X_{v_1}(t)$  are continuous functions of  $t$ , the solutions of the above time-varying, linear systems of ODEs can be written as ( $n_1 = 1, \dots, N$ ):

$$V_{\nu n_1}^{X^0}(t) = \sum_{v_1=1}^N \Phi_{\nu v_1}^{X^0}(t; t_0) \delta_{v_1 n_1} = \Phi_{\nu n_1}^{X^0}(t; t_0), \quad \nu = 1, \dots, N, \quad (3.11)$$

where  $\Phi_{\nu n_1}^{X^0}(t; t_0)$  denote the *state-transition matrix*, [81], of the IVP (3.10).

### 3.3.2 Calculation of the variational derivatives $V_{m\ell}^{\Xi(s)}$

In analogy with the above procedure, to calculate the variational derivative  $\delta \dot{X}_\nu(t)/\delta \Xi_{n_2}(s)$  we apply the Volterra derivative operator  $\delta \bullet / \delta \Xi_{n_2}(s)$ ,  $s \in [t_0, t]$ , to both sides of equations (3.9a,b). Assuming that the chain rule holds true for the Volterra derivatives, we derive the following problems:

$$\frac{\delta \dot{X}_\nu(t)}{\delta \Xi_{n_2}(s)} = \sum_{\nu_1=1}^N \frac{\partial h_\nu(\mathbf{X}(t), t)}{\partial X_{\nu_1}(t)} \frac{\delta X_{\nu_1}(t)}{\delta \Xi_{n_2}(s)} + \frac{\delta \Xi_\nu(t)}{\delta \Xi_{n_2}(s)}, \quad t_0 < s, t \quad (3.12a)$$

$$\frac{\delta X_\nu(t_0)}{\delta \Xi_{n_2}(s)} = 0, \quad \nu = 1, \dots, N. \quad (3.12b)$$

Under the assumption that the derivative operators  $\delta \bullet / \delta \Xi_{n_2}(s)$  and  $d \bullet / dt$  are interchangeable, and using the well-known result  $\delta \Xi_\nu(t)/\delta \Xi_{n_2}(s) = \delta_{\nu n_2} \delta(t-s)$ , equation (3.12a) takes the form:

$$\frac{d}{dt} \frac{\delta X_\nu(t)}{\delta \Xi_{n_2}(s)} = \sum_{\nu_1=1}^N \left( \frac{\partial h_\nu(\mathbf{X}(t), t)}{\partial X_{\nu_1}(t)} \right) \frac{\delta X_{\nu_1}(t)}{\delta \Xi_{n_2}(s)} + \delta_{\nu n_2} \delta(t-s), \quad n_2 = 1, \dots, N. \quad (3.12a')$$

**Remark 2:** It can be shown that the assumptions made in the derivation of equations (3.12a') and (3.10a) are valid under reasonable technical conditions on the analytical structure of the studied equations and the excitations. In the present work we focus on the essential steps of the derivation, assuming that the appropriate technical conditions are satisfied.

Equation (3.12a') is not in a form convenient for further study and solution. It can be reformulated as a linear system in the standard form by invoking a *causality argument*, as in [44, 77]. Any variation of the excitation,  $\delta \Xi_{n_2}(s)$ , at the time  $s$ , cannot result in a variation of the response,  $\delta X_{\nu_1}(t)$ , at any previous time  $t < s$ , implying  $\delta X_\nu(t)/\delta \Xi_{n_2}(s) = 0$  for  $t < s$  and any  $n_2, \nu_1 \in \{1, \dots, N\}$ . Thus, we have

$$V_{\nu n_2}^{\Xi(s)}(\tau) = \frac{\delta X_\nu(\tau)}{\delta \Xi_{n_2}(s)} \equiv \frac{\delta \mathcal{X}_\nu[\mathbf{X}^0(\theta); \Xi(\bullet)|_s^\tau; \theta]}{\delta \Xi_{n_2}(s)} = 0, \quad \text{for any } \tau \in [t_0, s]. \quad (3.13)$$

Based on equation (3.13), we reformulate equation (3.12a') in integral form, integrating with respect to time over the interval  $[s-\varepsilon, t]$ , for small  $\varepsilon > 0$ :

$$\frac{\delta X_\nu(t)}{\delta \Xi_{n_2}(s)} = \sum_{\nu_1=1}^N \int_{s-\varepsilon}^t \left( \frac{\partial h_\nu(\mathbf{X}(\tau), \tau)}{\partial X_{\nu_1}(\tau)} \right) \frac{\delta X_{\nu_1}(\tau)}{\delta \Xi_{n_2}(s)} d\tau + \delta_{\nu n_2} \underbrace{\int_{s-\varepsilon}^t \delta(\tau-s) d\tau}_{=1}. \quad (3.12a'')$$

Integrating from  $s - \varepsilon$  (up to  $t$ ) is consistent with equation (3.13), and helps us to formulate a well-defined integral of the delta function (equals to 1), avoiding having the singularity point at the lower integration limit. By taking the limit as  $\varepsilon \rightarrow 0$ , we obtain a Volterra integral equation of the second kind, which for  $n_2 \in \{1, \dots, N\}$  is equivalent to the following IVP [82]:

$$\frac{d}{dt} V_{\nu n_2}^{\Xi(s)}(t) = \sum_{\nu_1=1}^N \left( \frac{\partial h_{\nu}(\mathbf{X}(t), t)}{\partial X_{\nu_1}(t)} \right) V_{\nu_1 n_2}^{\Xi(s)}(t), \quad t > s, \quad (3.14a)$$

$$V_{\nu n_2}^{\Xi(s)}(s) = \delta_{\nu n_2}, \quad \nu = 1, \dots, N, \quad (3.14b)$$

System (3.14), being in the standard form, permits us to write its solution in the form:

$$V_{\nu n_2}^{\Xi(s)}(t) = \sum_{\nu_1=1}^N \Phi_{\nu \nu_1}^{\Xi}(t; s) \delta_{\nu_1 n_2} = \Phi_{\nu n_2}^{\Xi}(t; s), \quad \nu, n_2 = 1, \dots, N, \quad (3.15)$$

where  $\Phi_{\nu n_2}^{\Xi}(t; s)$  is the *state-transition matrix* of the IVP (3.14).

### 3.4 Final form of the transformed SLE and further discussion

To formulate the final form of the SLE, we restore the stochastic argument and substitute in the transformed SLE (3.8) the solutions  $V_{\nu n_1}^{X^0}(t; \theta)$ ,  $V_{\nu n_2}^{\Xi(s)}(t; \theta)$ , given by equations (3.11) and (3.15), respectively. Then we obtain the following equation:

$$\begin{aligned} & \frac{\partial f_{X(t)}(\mathbf{x})}{\partial t} + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left[ \left( h_n(\mathbf{x}) + m_{\Xi_n(\cdot)}(t) \right) f_{X(t)}(\mathbf{x}) \right] = \\ & + \sum_{n=1}^N \sum_{\nu=1}^N \frac{\partial}{\partial x_n} \frac{\partial}{\partial x_\nu} \sum_{n_1=1}^N C_{X_{n_1}^0 \Xi_n(\cdot)}(t) \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \Phi_{\nu n_1}^{X^0}(t; t_0, \theta) \right] + \\ & + \sum_{n=1}^N \sum_{\nu=1}^N \frac{\partial}{\partial x_n} \frac{\partial}{\partial x_\nu} \sum_{n_2=1}^N \int_{t_0}^t C_{\Xi_n(\cdot) \Xi_{n_2}(\cdot)}(t, s) \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \Phi_{\nu n_2}^{\Xi}(t; s, \theta) \right] ds. \end{aligned} \quad (3.16)$$

Equation (3.16) is structurally identical to equation (3.8). The difference is that the variational derivatives (3.7a,b) in (3.8) have been expressed by using the state-transition matrices which realize the solutions of the variational problems (3.10a,b) and (3.14a,b). The explicit calculation (or a good analytic approximation) of the state-transition matrices is an essential step to move forward. The treatment of the latter varies among authors, see e.g. [43, 44]. To that end, we prioritize the analytic treatment of the state-transition matrices, as expressed by the Peano-Baker [81] and Magnus [83, 84] series representations, see Appendix B. This perspective permits us to derive new genFPKE for nonlinear systems of RDE, outperforming existing ones (see Section 5). However, before proceeding to the derivation of our novel pdf-evolution equation, it seems appropriate to present some simple applications of the transformed SLE.

#### 4. First, simple applications of the transformed SLE

In this Section, we shall first derive an equation for the evolution of the response pdf of a linear system, under colored Gaussian excitation. The obtained model equation encompasses the complete (transient and long-term) probabilistic behavior of the system, is analytically solvable, and provides us with a simple model equation for testing numerical schemes.

##### 4.1 Pdf-evolution equation for linear systems, under coloured noise excitation

Assuming that the  $h_n$  functions in equations (2.1a), are linear in  $\mathbf{X}$ ,

$$h_n(\mathbf{X}(t; \theta)) = \sum_{m=1}^N \eta_{nm}(t) X_m(t; \theta), \quad n = 1, 2, \dots, N, \quad (4.1)$$

the corresponding system of RDE becomes *linear*. In order to specify the general equation (3.16) to the present case (as well as to any of the cases studied subsequently), we have to calculate the average terms of its right-hand side, which are concisely written as follows:

$$\mathcal{G}_{v_{n_1}}(t; t_0) = \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \Phi_{v_{n_1}}^{\mathbf{X}_0}(t; t_0, \theta) \right], \quad (4.2a)$$

$$\mathcal{G}_{v_{n_2}}(t; s) = \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \Phi_{v_{n_2}}^{\Xi}(t; s, \theta) \right]. \quad (4.2b)$$

To calculate the above averages, first we need to determine the state-transition matrices  $\Phi^{\mathbf{X}_0}$  and  $\Phi^{\Xi}$ , which are defined path-wisely (and thus, in general, they depend on the stochastic argument  $\theta$ ). In the linear case, the common system matrix of the variational problems (3.10) and (3.14),  $\partial h_n(\mathbf{X}(t; \theta), t) / \partial X_m = \eta_{nm}(t)$ , becomes independent of  $\mathbf{X}(t; \theta)$ . Thus, the variational problems (3.10) and (3.14) become *deterministic, time-varying* linear systems of ODEs. This allows us to calculate the averages (4.2a,b) directly, since the matrices  $\Phi^{\mathbf{X}_0}$  and  $\Phi^{\Xi}$  are factored out of the expected value operator, obtaining the expressions:

$$\mathcal{G}_{v_{n_1}}(t; t_0) = \Phi_{v_{n_1}}^{\mathbf{X}_0}(t; t_0) f_{X(t)}(\mathbf{x}), \quad \mathcal{G}_{v_{n_2}}(t; s) = \Phi_{v_{n_2}}^{\Xi}(t; s) f_{X(t)}(\mathbf{x}). \quad (4.3a,b)$$

Then, by substituting equations (4.3a,b) into equation (3.16), we obtain the following *linear pdf-evolution* equation:

$$\begin{aligned} \frac{\partial f_{X(t)}(\mathbf{x})}{\partial t} + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left[ \left( h_n(\mathbf{x}) + m_{\Xi_n(\cdot)}(t) \right) f_{X(t)}(\mathbf{x}) \right] = \\ = \sum_{n=1}^N \sum_{v=1}^N \left( \mathcal{D}_{v_n}^{\mathbf{X}_0 \Xi(\cdot)}(t) + \mathcal{D}_{v_n}^{\Xi(\cdot) \Xi(\cdot)}(t) \right) \frac{\partial}{\partial x_n} \frac{\partial}{\partial x_v} f_{X(t)}(\mathbf{x}), \end{aligned} \quad (4.4)$$

where the diffusion coefficients on the right-hand side of equation (4.4), are given by:

$$\mathcal{D}_{v_n}^{\mathbf{X}_0 \Xi(\cdot)}(t; t_0) = \sum_{n_1=1}^N C_{X_{n_1} \Xi_n(\cdot)}^{\mathbf{X}_0}(t) \Phi_{v_{n_1}}^{\mathbf{X}_0}(t; t_0), \quad (4.5a)$$

$$\mathcal{D}_{\nu n}^{\Xi(\cdot)\Xi(\cdot)}(t) = \sum_{n_2=1}^N \int_{t_0}^t C_{\Xi_n(\cdot)\Xi_{n_2}(\cdot)}(t,s) \Phi_{\nu n_2}^{\Xi}(t;s) ds. \quad (4.5b)$$

Note that explicit closed-form expression for the matrices  $\Phi^{X_0}$  and  $\Phi^{\Xi}$  are not generally available for *time-varying* variational problems. A discussion on the main representations of state-transition matrices and their approximations is presented in Appendix B. In the case of a system of RDE with constant coefficients, i.e.  $\eta_{nm}(t) = \eta_{nm}$ , the common system matrix of the variational problems becomes constant, namely  $(\mathbf{J}^h)_{nm} := \partial h_n(\mathbf{X}(t;\theta), t) / \partial X_m = \eta_{nm}$ , and the corresponding state-transition matrices  $\Phi^{X_0}$  and  $\Phi^{\Xi}$  take the form of matrix exponentials ([81], Section 1.5), namely,

$$\Phi_{\nu n_1}^{X_0}(t; t_0) = \left( \exp\left((t - t_0) \mathbf{J}^h\right) \right)_{\nu n_1}, \quad \Phi_{\nu n_2}^{\Xi}(t; s) = \left( \exp\left((t - s) \mathbf{J}^h\right) \right)_{\nu n_2}. \quad (4.6a,b)$$

Equation (4.4) is a linear transport-diffusion PDE for the evolution of  $f_{X(t)}(\mathbf{x})$ , which has also been presented in [33], for the case of a system with constant coefficients. This equation, supplemented by the initial condition:

$$f_{X(t_0)}(\mathbf{x}) = f_0(\mathbf{x}) \quad (= \text{general Gaussian}), \quad (4.7a)$$

and the additional data (coefficient functions)

$$\mathbf{m}_{\Xi(\cdot)}(t), \quad \mathbf{C}_{X_0 \Xi(\cdot)}(t), \quad (4.7b)$$

can be solved analytically via order reduction, using Fourier transform and the method of characteristics. Its solution is presented in [34]. On the other hand, it is well known that a linear system under Gaussian excitation yields a Gaussian response, which permits us to construct the response pdf by solving the corresponding moment problem. The direct analytic solution of PDE (4.4), for system with constant coefficients, coincides with the solution obtained by means of the moments [34], a fact that provides a first justification of the present approach.

#### 4.1.1 *The case of a linear damped oscillator*

Here we elaborate pdf-evolution equation (4.4) for the case of a damped harmonic oscillator, driven by a colored Gaussian excitation. The corresponding dynamical equation is

$$\ddot{X}(t; \theta) + 2\zeta \omega_0 \dot{X}(t; \theta) + \omega_0^2 X(t; \theta) = \Xi(t; \theta), \quad (4.8)$$

where  $\zeta$  denotes the dimensionless *damping coefficient* and  $\omega_0$  is the *natural frequency* of the undamped oscillator. Introducing the state-vector  $(X_1, X_2)^T = (X, \dot{X})^T$ , the oscillator is expressed in the form of the RDE system (2.1), with  $N = 2$ . The  $h_n$  functions in (2.1a) are specified in the forms:

$$h_1(\mathbf{X}(t; \theta), t) = X_2(t; \theta), \quad h_2(\mathbf{X}(t; \theta), t) = -\omega_0^2 X_1(t; \theta) - 2\zeta \omega_0 X_2(t; \theta). \quad (4.9a,b)$$

In this case, the excitation vector  $\Xi(t; \theta) = (\Xi_1, \Xi_2)^\top(t; \theta)$  is not a full vector, since the first equation of the system is unforced,  $\Xi_1 = 0$ . Therefore, the cross-covariances  $C_{X_n^0 \Xi_1(\cdot)}$  and auto-covariances  $C_{\Xi_n(\cdot) \Xi_1(\cdot)}$  vanish, for  $n = 1, 2$ , resulting in the zeroing of the diffusion coefficients  $\mathcal{D}_{\nu 1}^{X_0 \Xi(\cdot)}$ ,  $\mathcal{D}_{\nu 1}^{\Xi(\cdot) \Xi(\cdot)}$ , for  $\nu = 1, 2$ . To specify the remaining diffusion coefficients, equations (4.5a,b), we calculate the state transition matrices  $\Phi^{X_0}$  and  $\Phi^\Xi$ , given by (4.6a,b), respectively. Taking into account that, in this case, the system matrix for the variational problems is

$$\mathbf{J}^h = \nabla(h_1, h_2) = \begin{bmatrix} 0 & 1 \\ -\omega_0^2 & -2\zeta\omega_0 \end{bmatrix},$$

and restricting ourselves to the underdamped case,  $0 < \zeta < 1$ , we obtain (see e.g. [33] Sec.4, [85] or [86])

$$\Phi^\Xi(t, s) = e^{(t-s)\mathbf{J}^h} = e^{-a(t-s)} \sin(\gamma(t-s)) \begin{bmatrix} \cot(\gamma(t-s)) + a/\gamma & 1/\gamma \\ -\omega_0^2/\gamma & \cot(\gamma(t-s)) - a/\gamma \end{bmatrix}, \quad (4.10)$$

where  $a = \zeta\omega_0$  and  $\gamma = \omega_0(1 - \zeta^2)^{1/2}$ . By setting  $s = t_0$  in the above equation, we also obtain the matrix  $\Phi^{X_0}$ . Using equation (4.10), the diffusion coefficients (4.5a,b) are completely determined, and the right-hand side of equation (4.4) takes the form:

$$\sum_{\nu=1}^2 \left( \mathcal{D}_{\nu 2}^{X_0 \Xi(\cdot)}(t) + \mathcal{D}_{\nu 2}^{\Xi(\cdot) \Xi(\cdot)}(t) \right) \partial_{x_2 x_\nu} f_{X(t)}(\mathbf{x}) = \sum_{\nu=1}^2 U^{(\nu)}(t; t_0) \partial_{x_2 x_\nu} f_{X(t)}(\mathbf{x}), \quad (4.11)$$

where the coefficient functions  $U^{(\nu)}(t; t_0)$  are given by the following equations

$$U^{(1)}(t; t_0) = C_{X_1^0 \Xi(\cdot)}(t) \Phi_{11}^{X_0}(t, t_0) + C_{X_2^0 \Xi(\cdot)}(t) \Phi_{12}^{X_0}(t, t_0) + \int_{t_0}^t C_{\Xi(\cdot) \Xi(\cdot)}(t, s) \Phi_{12}^\Xi(t, s) ds, \quad (4.12a)$$

$$U^{(2)}(t; t_0) = C_{X_1^0 \Xi(\cdot)}(t) \Phi_{21}^{X_0}(t, t_0) + C_{X_2^0 \Xi(\cdot)}(t) \Phi_{22}^{X_0}(t, t_0) + \int_{t_0}^t C_{\Xi(\cdot) \Xi(\cdot)}(t, s) \Phi_{22}^\Xi(t, s) ds. \quad (4.12b)$$

Equations (4.10-4.12b), completely specifies the corresponding equation (4.4) for a damped harmonic oscillator. Further, the latter can be written in the form

$$\partial f_{X(t)}(\mathbf{x}) / \partial t + L[f_{X(t)}(\mathbf{x})] = 0,$$

where  $L[\cdot]$  is a linear second order partial differential operator of the form:

$$\begin{aligned}
L[\bullet] = & -U^{(1)}(t; t_0) \partial_{x_2 x_1} \bullet - U^{(2)}(t; t_0) \partial_{x_2 x_2} \bullet + \\
& + x_2 \partial_{x_1} \bullet + \left( m_{\Xi(\cdot)}(t) - \omega_0^2 x_1 - 2\zeta \omega_0 x_2 \right) \partial_{x_2} \bullet - 2\zeta \omega_0 \bullet.
\end{aligned} \tag{4.13}$$

For comparison purposes, we note that, in the case of white noise excitation, equation (4.4) becomes the standard FPKE, and the operator  $L[\bullet]$  takes the form

$$L_{\text{FPK}}[\bullet] = -D(t) \partial_{x_2 x_2} \bullet + x_2 \partial_{x_1} \bullet + \left( -\omega_0^2 x_1 - 2\zeta \omega_0 x_2 \right) \partial_{x_2} \bullet - 2\zeta \omega_0 \bullet,$$

where  $D(t)$  is the noise intensity of the excitation  $\Xi(t; \theta)$ .

**Remark 3.** The operator (4.13) is not a standard parabolic operator, in the sense that it is asymmetric with respect to the second-order derivatives (the pure diffusive part). More precisely, one of the second and one of the mixed partial derivatives are lacking in the right-hand side of equation (4.13).

Numerical results for an underdamped *linear* oscillator under colored Gaussian excitation are presented, as a benchmark problem, in the **Supplementary Material**. The linear pdf-evolution equation (4.4), corresponding to this case, is solved numerically by means of a partition of unity finite element scheme, and the approximated response 2D and marginals 1D densities are calculated and nicely compared with the known analytic solutions, and MC simulations. This is a first test of validity for the main elements of the numerical scheme, which is also used for the solution of the nonlinear case in Sec. 6, as well as an assessment of the MC simulation procedure.

#### 4.2 *The case of white-noise excitation. An alternative derivation of the classical FPKE*

Under the assumption of a *white noise Gaussian* excitation, we have that:

$$m_{\Xi(\cdot)}(t) = \mathbf{0}, \quad \mathbf{C}_{\Xi(\cdot)\Xi(\cdot)}^{\text{WN}}(t, s) = 2\mathbf{D}(t) \delta(t-s), \tag{4.14a,b}$$

where  $\mathbf{D}(t)$  is a positive-definite matrix which is called the noise intensity matrix. Assuming further

$$\mathbf{C}_{X_0 \Xi(\cdot)}(t) = \mathbf{0}, \tag{4.14c}$$

and substituting equations (4.14) in equation (3.16), the later simplifies in the following form:

$$\begin{aligned}
\frac{\partial f_{X(t)}(\mathbf{x})}{\partial t} + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left( h_n(\mathbf{x}) f_{X(t)}(\mathbf{x}) \right) = \\
= \sum_{n=1}^N \sum_{v=1}^N \frac{\partial^2}{\partial x_n \partial x_v} \sum_{n_2=1}^N 2D_{nn_2}(t) \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) B_{vn_2}(t) \right],
\end{aligned} \tag{4.15a}$$

where

$$B_{vn_2}(t) = \int_{t_0}^t \delta(t-s) \Phi_{vn_2}^{\Xi}(t; s, \theta) ds. \tag{4.15b}$$

To finish the derivation of the classical FPKE, we have to calculate the integral  $B_{vn_2}(t)$ . A technical difficulty in this calculation arises from the fact that the integrand contains a delta function whose singular point coincides with the upper limit of integration. Such a calculation does not have a standard mathematical meaning and should be performed as a limiting calcu-

lation, guided by the underlying physics. In this connection, we regularize the integral, representing the delta function by a *delta family* of smooth functions  $\delta_\varepsilon(t-s)$ , which recovers the delta function as the weak limit for  $\varepsilon \downarrow 0$ :

$$\delta(t-s) = \lim_{\varepsilon \downarrow 0} \delta_\varepsilon(t-s) = \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon} q\left(\frac{t-s}{\varepsilon}\right), \quad (4.16)$$

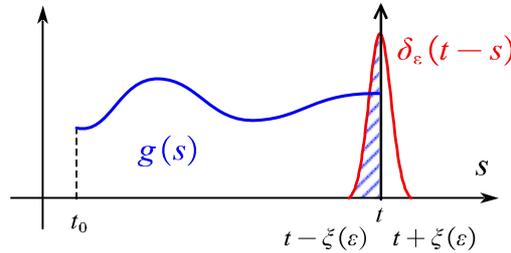
where  $q(\cdot)$  is any non-negative, normalized smooth function (kernel), supported around zero, [87]. Under these considerations, equation (4.14b) is written as

$$\mathbf{C}_{\Xi(\cdot)\Xi(\cdot)}^{\text{WN}}(t, s) = \lim_{\varepsilon \downarrow 0} \mathbf{C}_{\Xi(\cdot)\Xi(\cdot)}^{(\varepsilon)}(t, s) = 2\mathbf{D}(t) \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon} q\left(\frac{t-s}{\varepsilon}\right). \quad (4.14b')$$

Since any autocovariance  $\mathbf{C}_{\Xi(\cdot)\Xi(\cdot)}^{(\varepsilon)}(t, s) = \mathbf{C}_{\Xi(\cdot)\Xi(\cdot)}^{(\varepsilon)}(t-s)$  is an even function, the kernel function  $q(\cdot)$ , defining the delta function in this case, must be an even function as well. This requirement implies, for any continuous function  $g(\cdot)$ , that:

$$\lim_{\varepsilon \downarrow 0} \int_{t_0}^t \delta_\varepsilon(t-s) g(s) ds = \lim_{\varepsilon \downarrow 0} \left( g(\tilde{t}(\varepsilon)) \int_{t-\xi(\varepsilon)}^t \delta_\varepsilon(t-s) ds \right) = \frac{1}{2} g(t), \quad (4.17)$$

where  $t - \xi(\varepsilon) < \tilde{t}(\varepsilon) < t$ . The first equality in the above equation is implied by the mean value theorem, and the second one by the fact that  $\lim_{\varepsilon \downarrow 0} g(\tilde{t}(\varepsilon)) = g(t)$  and the restriction of the integration of the symmetric  $\delta_\varepsilon(t-s)$  to the half-interval, see Figure 1.



**Figure 1:** Geometrical interpretation of the integral  $\lim_{\varepsilon \downarrow 0} \int_{t_0}^t \delta_\varepsilon(t-s) g(s) ds$

Applying equation (4.17), the calculation of the integral  $B_{\nu n_2}(t)$  is now straightforward. Indeed, the *state-transition matrix*  $\Phi(t, s; \theta)$  is a continuous function with respect to both arguments  $t, s$ , and  $\lim_{s \rightarrow t} \Phi(t, s; \theta) = \mathbf{I}$ , where  $\mathbf{I}$  indicates the identity matrix. Thus, we readily obtain  $B_{\nu n_2}(t) = (1/2) \delta_{\nu n_2}$ . Finally, by substituting  $B_{\nu n_2}(t)$  in (4.15a), using the

identity  $\sum_{n_2=1}^N \mathbf{D}_{nn_2}(t) \delta_{\nu n_2} = \mathbf{D}_{n\nu}(t)$ , and recalling equation (2.2), we derive

$$\frac{\partial f_{X(t)}(\mathbf{x})}{\partial t} + \sum_{n=1}^N \frac{\partial}{\partial \mathbf{x}_n} [h_n(\mathbf{x}) f_{X(t)}(\mathbf{x})] = \sum_{n=1}^N \sum_{\nu=1}^N \mathbf{D}_{n\nu}(t) \frac{\partial^2 f_{X(t)}(\mathbf{x})}{\partial \mathbf{x}_n \partial \mathbf{x}_\nu}, \quad (4.18)$$

which is the classical **Fokker-Planck-Kolmogorov (FPK) equation** [5, 88], corresponding to a nonlinear system of RDEs, excited by additive Gaussian white noise.

**Remark 4.** It is interesting to note that the above derivation of the FPKE is straightforward, concise, and clear. This is due to the explicit consideration of the non-locality of the problem, via the SLE. The present approach permits us to circumvent the need to resort to the (somewhat artificial) infinite-dimensional kinetic equation (Kramer-Moyal expansion; [89] pp. 43-47, [90] Sec. 7.2.3), or to the purely analytic treatment of Kolmogorov (see, e.g., [89] pp. 47-49, [8] Sec. 3.4-3.5.2). Here, the standard FPKE results naturally from the transformed SLE (after using the NF Theorem) via the assumption of delta correlation for the excitation, by only using equation (4.17). This apparently exact result can also be considered as an *automatic current-time approximation*, since it forcefully excludes (by its delta-type definition) any memory effects carried over by the transition matrix  $\Phi^\Xi$ ; see equation (4.15b).

#### 4.3 *The small correlation time (SCT) pdf-evolution equation*

In this section, we derive a SCT pdf-evolution equation for a nonlinear system of RDE, under additive Gaussian coloured noise excitation. The meaning of the SCT approximation is that the significant effects of  $C_{X_{n_1}^0 \Xi_{n_2}(\cdot)}(t)$  and  $C_{\Xi_{n_1}(\cdot) \Xi_{n_2}(\cdot)}(t, s)$  are concentrated near  $t_0$  and near the current time  $t$ , respectively. The derivation presented herein is easy and straightforward, due to the analytic approximations of the state-transition matrices  $\Phi^{X^0}$  and  $\Phi^\Xi$ .

Approximating  $\Phi^\Xi$  by using the first two terms of the Peano Baker series (see Appendix B), we obtain

$$\Phi^\Xi(t; s, \theta) \approx I + \int_s^t J^h(X(u; \theta), u) du . \quad (4.19)$$

Introducing a *current-time approximation* for the integral in the above expression, we get

$$\Phi^\Xi(t; s, \theta) \approx I + J^h(X(t; \theta), t)(t - s) . \quad (4.20)$$

The same treatment applies to the matrix  $\Phi^{X^0}$ , and the corresponding final approximation is given by equation (4.20) with  $s = t_0$ . By using these approximations for the matrices  $\Phi^{X^0}$  and  $\Phi^\Xi$ , the expected value operators in equations (4.2a,b) can be easily calculated, resulting in their localization at the current time  $t$ :

$$\mathcal{G}_{v_{n_1}}(t; t_0) = I_{v_{n_1}} f_{X(t)}(\mathbf{x}) + \left( J^h(\mathbf{x}, t) \right)_{v_{n_1}} f_{X(t)}(\mathbf{x})(t - t_0), \quad (4.21a)$$

$$\mathcal{G}_{v_{n_2}}(t; s) = I_{v_{n_2}} f_{X(t)}(\mathbf{x}) + \left( J^h(\mathbf{x}, t) \right)_{v_{n_2}} f_{X(t)}(\mathbf{x})(t - s). \quad (4.21b)$$

Via the above expressions, the transformed SLE (3.16) takes the form:

$$\begin{aligned} \frac{\partial f_{X(t)}(\mathbf{x})}{\partial t} + \sum_{n=1}^N \frac{\partial}{\partial x_n} \left[ \left( h_n(\mathbf{x}) + m_{\Xi_n(\cdot)}(t) \right) f_{X(t)}(\mathbf{x}) \right] = \\ = \sum_{n=1}^N \sum_{v=1}^N \frac{\partial}{\partial x_n} \frac{\partial}{\partial x_v} \left[ \left( \mathcal{D}_{v_n}^{X_0 \Xi(\cdot)}[\mathbf{x}, t] + \mathcal{D}_{v_n}^{\Xi(\cdot) \Xi(\cdot)}[\mathbf{x}, t] \right) f_{X(t)}(\mathbf{x}) \right], \end{aligned} \quad (4.22)$$

where

$$\mathcal{D}_{v_n}^{X_0 \Xi(\cdot)}[\mathbf{x}, t] = \sum_{n_1=1}^N C_{X_{n_1}^0 \Xi_n(\cdot)}(t) \left( I_{v_{n_1}} + \left( \mathbf{J}^h(\mathbf{x}, t) \right)_{v_{n_1}} (t - t_0) \right), \quad (4.23a)$$

$$\mathcal{D}_{v_n}^{\Xi(\cdot) \Xi(\cdot)}[\mathbf{x}, t] = \sum_{n_2=1}^N \int_{t_0}^t C_{\Xi_{n_2}(\cdot) \Xi_{n_2}(\cdot)}(t, s) \left( I_{v_{n_2}} + \left( \mathbf{J}^h(\mathbf{x}, t) \right)_{v_{n_2}} (t - s) \right) ds \quad (4.23b)$$

To compare equation (4.22) with other existing ones, first we have to impose the assumptions of *zero-mean* excitations,  $m_{\Xi_n(\cdot)}(t) = 0$ , and  $\mathcal{D}_{v_n}^{X_0 \Xi(\cdot)}[\mathbf{x}, t] = 0$  (initial data uncorrelated with the excitation). Terms containing the above two functions do not appear in existing literature, probably because the extended NF theorem, equation (3.5), was not available. Further, a comparison of equation (4.22) with existing genFPKE is not straightforward since in the literature the results are usually given for the multiplicative excitation, leaving the additive case as a special one (obtained after some analytical manipulations). It can be shown that the additive excitation versions of the pdf-evolution equation derived by San Miguel and Sancho in 1980 [45], and Dekker in 1982 [44], degenerates to equation (4.22). In the latter work, the equation has been derived in a more laborious way, via the correlation time expansion method. Moreover, equation (4.22) can be also deduced from the results of references [47, 91] obtained by the ordered cumulant expansion method. In comparison with our derivation, the main methodological difference lies in the use of the analytic approximation of the Volterra derivatives  $V_{v_{n_2}}^{\Xi(s)}(t)$ . It seems that our approach provides an easier derivation for equation (4.22), pertaining to the additive excitation by colored noise.

## 5. A novel pdf-evolution equation for $N$ -dimensional nonlinear systems

In this section we present the derivation of our novel response pdf-evolution equation, announced in equation (2.6), which is based on the separation of the (instantaneous) mean value of the response, from its random fluctuations. This separation is reflected at the level of the state-transition matrices  $\Phi^{X_0}$  and  $\Phi^{\Xi}$ , via an appropriate matrix decomposition. To motivate the method and facilitate its understanding, it is useful to highlight the main steps first in the case of a scalar RDE (one-dimensional case). The latter case has been presented in [25], by using a more complicated procedure.

### 5.1 Motivation: *Applying the novel closure to a scalar RDE*

In the scalar case, the transition matrix  $\Phi^{\Xi}$  has the form of an exponential function, thus  $\mathcal{G}(t; s)$ , equation (4.2b), is now a scalar quantity, which takes the form:

$$\mathcal{G}(t; s) \equiv \mathbb{E}^\theta \left[ \delta(x - X(t; \theta)) \exp \left( \int_s^t h'(X(u; \theta), u) du \right) \right]. \quad (5.1)$$

That is, the exponential function plays the role of the one-dimensional state-transition matrix,  $\Phi^\Xi(t; s, \theta)$ . The main idea is to decompose  $h'$  (which now is a scalar function) into its **mean** and **fluctuating** (around the mean value) part:

$$h'(X(t; \theta), t) = \mathbb{E}^\theta [h'(X(t; \theta), t)] + \Delta_{h'}(X(t; \theta), t). \quad (5.2)$$

where  $\Delta_{h'}(X(t; \theta), t) = h'(X(t; \theta), t) - R_{h'}[f_{X(t)}(\cdot), t]$ . We note that the instantaneous mean value of  $h'$  engages a generalized response moment,

$$\mathbb{E}^\theta [h'(X(t; \theta), t)] = \int_{\mathbb{R}} h'(x, t) f_{X(t)}(x) dx, \quad (5.3a)$$

which subsequently treated without any further simplification. This quantity is explicitly dependent on the unknown pdf at the time instant  $t$ . To highlight this dependence, we introduce the notation,

$$R_{h'}[f_{X(t)}(\cdot), t] := \mathbb{E}^\theta [h'(X(t; \theta), t)]. \quad (5.3b)$$

Substituting the decomposition (5.2) into the exponential function in equation (5.1), we obtain,

$$\exp \left( \int_s^t h'(X(u; \theta), u) du \right) = \exp \left( \int_s^t R_{h'}[f_{X(u)}(\cdot), u] du \right) \exp \left( \int_s^t \Delta_{h'}(X(u; \theta), u) du \right) \quad (5.4)$$

Introducing a current-time approximation in the second integral of the right-hand side of equation (5.4), which contains only the *fluctuating part*  $\Delta_{h'}(X(t; \theta), t)$ , we obtain

$$\exp \left( \int_s^t \Delta_{h'}(X(u; \theta), u) du \right) \approx \exp \left( \Delta_{h'}(X(t; \theta), t) (t - s) \right). \quad (5.5)$$

Substituting equation (5.4) into equation (5.1), utilizing equation (5.5), and factoring out of the expected value operator the deterministic exponential term, we obtain

$$\begin{aligned} \mathcal{G}(t; s) &= \exp \left( \int_s^t R_{h'}[f_{X(u)}(\cdot), u] du \right) \mathbb{E}^\theta \left[ \exp \left( \Delta_{h'}(X(t; \theta), t) (t - s) \right) \delta(x - X(t; \theta)) \right] = \\ &= \exp \left( \int_s^t R_{h'}[f_{X(u)}(\cdot), u] du \right) \exp \left( \Delta_{h'}(x, t) (t - s) \right) f_{X(t)}(x). \end{aligned} \quad (5.6)$$

The term  $\mathcal{G}(t; t_0)$  is obtained by setting  $s = t_0$  in equation (5.6). Simplifying the SLE (3.16) for  $N = 1$ , and substituting  $\mathcal{G}(t; t_0)$  and  $\mathcal{G}(t; s)$  in the latter, we obtain equation (2.6), for  $n = \nu = 1$ . The coefficients  $\mathcal{D}^{X_0 \Xi(\cdot)}$  and  $\mathcal{D}^{\Xi(\cdot) \Xi(\cdot)}$ , take now the form:

$$\begin{aligned} \mathcal{D}^{X_0 \Xi(\cdot)} [f_{X(\cdot)}(\cdot); x, t] &= \\ &= C_{X^0 \Xi(\cdot)}(t) \exp \left( \int_{t_0}^t R_{h'} [f_{X(u)}(\cdot), u] du \right) \exp \left( \Delta_{h'}(x, t) (t - t_0) \right), \end{aligned} \quad (5.7a)$$

$$\begin{aligned} \mathcal{D}^{\Xi(\cdot) \Xi(\cdot)} [f_{X(\cdot)}(\cdot); x, t] &= \\ &= \int_{t_0}^t C_{\Xi(\cdot) \Xi(\cdot)}(t, s) \exp \left( \int_s^t R_{h'} [f_{X(u)}(\cdot), u] du \right) \exp \left( \Delta_{h'}(x, t) (t - s) \right) ds. \end{aligned} \quad (5.7b)$$

Equation (2.6) (with coefficients (5.7a,b)) for the one-dimensional problem, has been first derived in [25], by using a more laborious methodology, based on Volterra series expansions. It is worthwhile to note that it has been extensively tested numerically [25] Sec. 4, [92], proving itself a very capable model for calculating the response pdf of scalar RDEs, far beyond the SCT excitation regime, up to non-dimensional correlation time 3 or more.

The extension of the above approach to a system of RDEs requires manipulations of the state-transition matrices  $\Phi^{X_0}$  and  $\Phi^\Xi$  and, also, the introduction of additional state-transition matrices associated with IVPs different than the variational problems (3.10) and (3.14). It is, therefore, expedient to enrich the notation used for the state-transition matrix  $\Phi = \Phi(t; t_0, \theta)$ , associated with the IVP

$$\dot{\mathbf{y}}_{[N \times 1]}(t; \theta) = \mathbf{A}_{[N \times N]}(\mathbf{X}(t; \theta), t) \mathbf{y}_{[N \times 1]}(t; \theta), \quad \mathbf{y}(t_0; \theta) = \mathbf{y}^0(\theta), \quad (\text{P})$$

as follows:  $\Phi = \Phi[\mathbf{A}](t; t_0, \theta)$ . Now, the underlying *system-matrix*  $\mathbf{A}$  of the IVP is also indicated in the notation. The function  $\mathbf{y}(t; \theta) = \Phi[\mathbf{A}](t; t_0, \theta) \mathbf{y}^0(\theta)$  solves problem (P) and, thus, by definition, the matrix  $\mathbf{Y}(t; \theta) = \Phi[\mathbf{A}](t; t_0, \theta)$  satisfies the *matrix differential equation*  $\dot{\mathbf{Y}}(t; \theta) = \mathbf{A}(\mathbf{X}(t; \theta), t) \mathbf{Y}(t; \theta)$ ,  $\mathbf{Y}(t_0) = \mathbf{I}$ . A visual interpretation of the dependencies in the notation  $\Phi[\mathbf{A}](t; s, \theta)$  is shown in Figure 2.

$$\Phi[\mathbf{A}](t; s, \theta) \rightarrow \text{solves} \rightarrow \begin{cases} \mathbf{Y}(t; \theta) = \mathbf{A}(\mathbf{X}(t; \theta), t) \mathbf{Y}(t; \theta), \\ \mathbf{Y}(s) = \mathbf{I} \end{cases}, \quad \mathbf{Y}, \mathbf{A} \in \mathbb{R}^{N \times N}$$

**Figure 2.** Visual explanation of the notation  $\Phi[\mathbf{A}](t; s, \theta)$ .

Using the above notation, equation (5.4), for the scalar case, can be rephrased, in terms of *one-dimensional state-transition matrices*, in the form

$$\Phi^\Xi[h'](t; s, \theta) = \Phi[R_{h'}](t; s, \theta) \Phi[\Delta_{h'}](t; s, \theta).$$

This equation implies a decomposition of the state-transition matrix, associated with the additive decomposition (5.2) and the exponential property  $e^{a(t)+b(t)} = e^{a(t)} e^{b(t)}$ . In the multidimensional case,

mensional case, the corresponding decomposition for exponential matrices does not hold in general ( $e^{A(t)+B(t)} \neq e^{A(t)}e^{B(t)}$ ) and further considerations should be made.

## 5.2 Generalization of the novel closure to the $N$ -dimensional case

In the multidimensional case, the system matrix of both variational problems, (3.10a) and (3.14a), is the Jacobian matrix of the vector function  $\mathbf{h}(X(t;\theta), t) = (h_1, \dots, h_N)(X(t;\theta), t)$ , see equation (2.1a), denoted as

$$\mathbf{J}^h := \mathbf{J}^h(X(t;\theta), t) = \nabla \mathbf{h}(X(t;\theta), t). \quad (5.8)$$

In this case, we again decompose the matrix  $\mathbf{J}^h(X(t;\theta), t)$ , in its mean value and its random fluctuations (around the mean value):

$$\mathbf{J}^h(X(t;\theta), t) := \mathbf{R}[f_{X(t)}(\cdot), t] + \mathcal{A}(X(t;\theta), t), \quad (5.9)$$

where

$$\mathbf{R}(t) \equiv \mathbf{R}[f_{X(t)}(\cdot), t] = \mathbb{E}^\theta[\mathbf{J}^h(X(t;\theta), t)] = \int_{\mathbb{R}^N} \mathbf{J}^h(x, t) f_{X(t)}(x) dx, \quad (5.10)$$

$$\mathcal{A}(X(t;\theta), t) = \mathbf{J}^h(X(t;\theta), t) - \mathbf{R}[f_{X(t)}(\cdot), t]. \quad (5.11)$$

Following the steps explained in the scalar case, we need to reflect the decomposition (5.9) on the level of the state-transition matrix  $\Phi^\Xi[\mathbf{J}^h]$ . To this end, we seek for a decomposition of  $\Phi^\Xi[\mathbf{J}^h]$ , in terms of the transition-matrix

$$\Phi[\mathbf{R}](t; s) \equiv \Phi[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s). \quad (5.12)$$

Herein we will make use of the simpler notation  $\Phi[\mathbf{R}](t; s)$  whenever the dependence of  $\mathbf{R}$  on the density field  $f_{X(\cdot)}(\cdot)$  is not important to be pointed out. It can be proved (see, e.g., [93] p. 219) that, under the additive decomposition (5.9), the following multiplicative decomposition holds true:

$$\Phi^\Xi[\mathbf{J}^h](t; s, \theta) = \Phi[\mathbf{R}](t; s) \Phi[\mathbf{B}](t; s, \theta), \quad (5.13a)$$

where the matrix  $\mathbf{B}(t, s; \theta)$  is expressed as:

$$\mathbf{B}(t, s; \theta) = \Phi^{-1}[\mathbf{R}](t; s) \mathcal{A}(X(t;\theta), t) \Phi[\mathbf{R}](t; s). \quad (5.13b)$$

The decomposition (5.13a) is the analog to equation (5.4), in the multidimensional case. By substituting equation (5.13a) into the non-local term (4.2b) and factoring the deterministic matrix  $\Phi[\mathbf{R}](t; s)$  out of the mean-value operator, we obtain

$$\mathcal{G}(t; s) = \Phi[\mathbf{R}](t; s) \mathbb{E}^\theta[\delta(\mathbf{x} - X(t;\theta)) \Phi[\mathbf{B}](t; s, \theta)]. \quad (5.14)$$

In equation (5.14),  $\mathcal{G}(t; s)$  represents the matrix whose components  $\mathcal{G}_{v_n}(t; s)$  are given by equation (4.2b). To implement our approximation scheme, we need an explicit representation of the matrix  $\Phi[\mathbf{B}](t; s, \theta)$ . To that end, we use the Magnus expansion of  $\Phi[\mathbf{B}](t; s, \theta)$  (see Appendix B, equations (B.3) and (B.4)), keeping only its first term, obtaining

$$\Phi[\mathbf{B}](t; s, \theta) \cong \exp\left(\int_s^t \mathbf{B}(u, s; \theta) du\right). \quad (5.15a)$$

Higher order terms of Magnus series can also be considered, leading to more complicated approximations. This issue will be studied in future work.

Combining equations (5.13b) and (5.15a), we get

$$\Phi[\mathbf{B}](t; s, \theta) \cong \exp\left(\int_s^t \Phi^{-1}[\mathbf{R}](t; s) \mathcal{A}(\mathbf{X}(u; \theta), u) \Phi[\mathbf{R}](t; s) du\right). \quad (5.15b)$$

Taking into account that the elements of the matrix  $\Phi[\mathbf{B}](t; s, \theta)$  are eventually multiplied by the elements of  $\mathbf{C}_{\Xi(\cdot), \Xi(\cdot)}(t, s)$  (see equation (3.16)), we understand that we need an approximation of the integral, in the right-hand side of equation (5.15b), which should become exact as  $s$  tends to  $t$ . The simplest approximation of this kind is the current-time approximation of the integrand (at  $t$ ), under which we perform the integration, obtaining

$$\begin{aligned} \Phi[\mathbf{B}](t; s, \theta) &\cong \exp\left(\Phi^{-1}[\mathbf{R}](t; s) \mathcal{A}(\mathbf{X}(t; \theta), t) \Phi[\mathbf{R}](t; s) (t-s)\right) = \\ &= \Phi^{-1}[\mathbf{R}](t; s) \exp\left(\mathcal{A}(\mathbf{X}(t; \theta), t) (t-s)\right) \Phi[\mathbf{R}](t; s). \end{aligned} \quad (5.16)$$

Again, better approximation can be considered by using Taylor expansion.

Now, by substituting equation (5.16) into equation (5.14), we obtain

$$\begin{aligned} \mathcal{G}(t; s) &= \mathbb{E}^\theta\left[\delta(\mathbf{x} - \mathbf{X}(t; \theta)) \exp\left(\mathcal{A}(\mathbf{X}(t; \theta), t) (t-s)\right)\right] \Phi[\mathbf{R}](t; s) = \\ &= \exp\left(\mathcal{A}(\mathbf{x}, t) (t-s)\right) \Phi[\mathbf{R}](t; s) f_{\mathbf{X}(t)}(\mathbf{x}), \end{aligned} \quad (5.17)$$

where the second equality is justified as follows:

$$\begin{aligned} \mathbb{E}^\theta\left[\delta(\mathbf{x} - \mathbf{X}(t; \theta)) \exp\left(\mathcal{A}(\mathbf{X}(t; \theta), t) (t-s)\right)\right] &= \\ &= \int_{\mathbb{R}^N} \delta(\mathbf{x} - \mathbf{u}) \exp\left(\mathcal{A}(\mathbf{u}, t) (t-s)\right) f_{\mathbf{X}(t)}(\mathbf{u}) d\mathbf{u} =, \\ &= \exp\left(\mathcal{A}(\mathbf{x}, t) (t-s)\right) f_{\mathbf{X}(t)}(\mathbf{x}). \end{aligned} \quad (5.18)$$

That is,  $\mathcal{A}(\mathbf{x}, t)$  is the matrix obtained by  $\mathcal{A}(\mathbf{X}(t; \theta), t)$  when replacing the random vector  $\mathbf{X}(t; \theta)$  by a deterministic vector  $\mathbf{x}$ .

The matrix  $\mathcal{G}(t; t_0)$ , whose components appear in equation (4.2a), is obtained by equation (5.17), after setting  $s = t_0$ . Note that equation (5.17) is the multidimensional analog of equation (5.6), of the scalar case.

Last, by substituting  $\mathcal{G}(t; s)$  and  $\mathcal{G}(t; t_0)$  into the *transformed SLE* (3.16), we obtain the new pdf-evolution equation (2.6), along with the exact forms of the diffusion coefficients, namely

$$\begin{aligned} \mathcal{D}_{vn}^{X_0 \Xi(\cdot)} [f_{X(\cdot)}(\cdot); \mathbf{x}, t] &= \\ &= \sum_{n_1=1}^N \sum_{k=1}^N C_{X_{n_1}^0 \Xi_{n_1}(\cdot)}(t) \Phi_{kn_1} [\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; t_0) \left( \exp(\mathbf{A}(\mathbf{x}, t)(t - t_0)) \right)_{vk}, \end{aligned} \quad (5.19a)$$

$$\begin{aligned} \mathcal{D}_{vn}^{\Xi(\cdot) \Xi(\cdot)} [f_{X(\cdot)}(\cdot); \mathbf{x}, t] &= \\ &= \sum_{n_2=1}^N \sum_{k=1}^N \int_{t_0}^t C_{\Xi_{n_2}(\cdot) \Xi_{n_2}(\cdot)}(t, s) \Phi_{kn_2} [\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s) \left( \exp(\mathbf{A}(\mathbf{x}, t)(t - s)) \right)_{vk} ds. \end{aligned} \quad (5.19b)$$

Equations (5.19) specify the expressions of the diffusion coefficients for our *novel one-time pdf-evolution equation* (2.6). The emergence of drift coefficients containing the mean values  $m_{\Xi_{n_1}(\cdot)}(t)$ , and of the diffusion coefficients  $\mathcal{D}_{vn}^{X_0 \Xi(\cdot)}$ , containing the cross-covariance of the initial data with the excitations, result by the use of the extended NF theorem, equation (3.3). To the best of our knowledge, such terms do not appear in other existing genFPKE.

### 5.3 Comparison with the SCT approximation

In this section we compare our novel pdf-evolution equation, which is (2.6) with diffusion coefficients given by equations (5.19a,b) (called *novel gFPKE*, for conciseness), with the SCT approximation, which is equation (2.6) with diffusion coefficients given by equations (4.23a,b). In this conjunction, we consider zero-mean excitation,  $m_{\Xi_{n_1}(\cdot)}(t) = 0$ , and uncorrelated excitation to the initial value,  $\mathcal{D}_{vn}^{X_0 \Xi(\cdot)}[\mathbf{x}, t] = 0$ . Then, the two equations have identical drift part and differ only in the diffusion coefficients matrix  $\mathcal{D}^{\Xi(\cdot) \Xi(\cdot)}$ . To compare the two cases, it is expedient to rewrite the components  $\mathcal{D}_{vn}^{\Xi(\cdot) \Xi(\cdot)}$  of the diffusion matrix, equations (5.19b) and (4.23b), in the following form:

$$\mathcal{D}_{vn}^{\Xi(\cdot) \Xi(\cdot)} [f_{X(\cdot)}(\cdot); \mathbf{x}, t] = \sum_{n_2=1}^N \int_{t_0}^t C_{\Xi_{n_2}(\cdot) \Xi_{n_2}(\cdot)}(t, s) \left\{ \begin{array}{l} D_{vn_2}^{\text{ngFPK}} [f_{X(\cdot)}(\cdot); \mathbf{x}, t, s] \\ D_{vn_2}^{\text{SCT}}(\mathbf{x}, t, s) \end{array} \right\} ds, \quad (5.20)$$

where

$$D_{vn_2}^{\text{ngFPK}}(f_{X(\cdot)}(\cdot); \mathbf{x}, t, s) = \sum_{k=1}^N \left( \exp(\mathbf{A}(\mathbf{x}, t)(t - s)) \right)_{vk} \Phi_{kn_2} [\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s) \quad (5.21a)$$

and

$$D_{vn_2}^{\text{SCT}}(\mathbf{x}, t, s) = I_{vn_2} + \left( \mathbf{J}^h(\mathbf{x}, t) \right)_{vn_2} (t - s). \quad (5.21b)$$

For both novel and SCT genFPKE, the diffusion coefficients are of the same integral form (5.20), differing only with respect to the matrix in bracket  $\{ \}$ , on the right-hand side. We

will now show how the matrix  $\mathbf{D}^{\text{ngFPK}}$  is reduced to the corresponding matrix  $\mathbf{D}^{\text{SCT}}$ , by means of a series of approximations. The first step is to approximate  $\Phi[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s)$  (in equations (5.21a)) via the first two terms of its Peano-Baker series expansion, namely,

$$\Phi[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s) \approx \mathbf{I} + \int_s^t \mathbf{R}[f_{X(u)}(\cdot), u] du. \quad (5.22a)$$

Then, we introduce a current-time approximation to the integral in the above equation, obtaining

$$\Phi[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s) \approx \mathbf{I} + \mathbf{R}[f_{X(t)}(\cdot), t](t - s). \quad (5.22b)$$

Since in the SCT derivation, the decomposition (5.9) of the matrix  $\mathbf{J}^h$  is not used, we have to come back to equation (5.17) and repeat the averaging by using equation (5.11):

$$\begin{aligned} & \mathbb{E}^\theta [\delta(\mathbf{x} - \mathbf{X}(t; \theta)) \exp(\mathcal{A}(\mathbf{X}(t; \theta), t)(t - s))] = \\ & = \mathbb{E}^\theta \left[ \delta(\mathbf{x} - \mathbf{X}(t; \theta)) \exp\left(\left(\mathbf{J}^h(\mathbf{X}(t; \theta), t) - \mathbf{R}[f_{X(t)}(\cdot), t]\right)(t - s)\right) \right] \\ & = \exp\left(\left(\mathbf{J}^h(\mathbf{x}, t) - \mathbf{R}[f_{X(t)}(\cdot), t]\right)(t - s)\right) f_{X(t)}(\mathbf{x}). \end{aligned}$$

This means that, in all manipulations made after calculating the averaging [in equation (5.17)], it is permissible to use the relation

$$\exp(\mathcal{A}(\mathbf{x}, t)(t - s)) = \exp\left(\left(\mathbf{J}^h(\mathbf{x}, t) - \mathbf{R}[f_{X(t)}(\cdot), t]\right)(t - s)\right).$$

It should be noted that this equation cannot be inferred by the decomposition (5.9) [or (5.11)]. It is a consequence of the specific localization (via the delta function  $\delta(\mathbf{x} - \mathbf{X}(t; \theta))$ ) performed in equation (5.17) via (5.18).

Now, by expanding the exponential matrix  $\exp(\mathcal{A}(\mathbf{x}, t)(t - s))$  in power series keeping only the two first terms, and exploiting equation (5.22b), we calculate the corresponding approximation of matrix  $\mathbf{D}^{\text{ngFPK}}$ , equation (5.21a), as follows

$$\begin{aligned} \mathbf{D}^{\text{ngFPK}}(f_{X(\cdot)}(\cdot); \mathbf{x}, t, s) & \approx \mathbf{I} + \mathbf{J}^h(\mathbf{x}, t)(t - s) + \\ & + \mathbf{R}[f_{X(t)}(\cdot), t] \left( \mathbf{J}^h(\mathbf{x}, t) - \mathbf{R}[f_{X(t)}(\cdot), t] \right) (t - s)^2. \end{aligned} \quad (5.23)$$

Neglecting the second order term with respect to  $(t - s)$ , equation (5.23) becomes equation (5.21b), which means that the novel FPK reduces to the SCT equation.

**Remark 5.** It is interesting to notice that, to derive the SCT approximate equation from our novel FPK, we have to neglect all memory effects included in  $\Phi[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]]$ , to simplify the exponential matrix  $\exp(\mathcal{A}(\mathbf{x}, t)(t - s))$ , and to neglect a second-order term, remaining after these simplifications. These facts are indicative of the amount of additional infor-

mation included in the novel FPK equation in comparison with the classical SCT approximation.

**Remark 6.** Further, it is easy to see that the novel gFPKE equation can be reduced to the pdf-evolution equation (4.4), in the case of linear systems, and to the standard FPKE (4.18), in the case of white noise excitation.

## 6. First numerical results

To test the validity of the proposed novel genFPKE (2.6), numerical simulations have been performed and briefly presented in this section. We consider the case of a randomly excited Duffing oscillator, and we compare its response pdf as obtained by solving the SCT genFPKE, the novel genFPKE and Monte Carlo (MC) simulations. The numerical method used for solving genFPKE employs: **i)** a partition of unity finite element method (PUFEM) for the discretization in the state space [60], **ii)** a Bubnov-Galerkin technique for deriving ODEs governing the evolution of the pdf and **iii)** a Crank-Nicolson scheme for solving the obtained ODEs in the time domain. Similar numerical methods have been used for solving the stationary FPKE [94, 95] and the transient FPKE [96, 97]. Details on the numerical treatment will be presented elsewhere. An additional test of validity of our numerical scheme and simulation procedure is presented in **Supplementary Material**, where results concerning the solution of the pdf-evolution equation corresponding to a linear oscillator are given. Since, in this case, analytical solution of the pdf evolution is available, we are able to test the efficiency of the corresponding MC simulations and the quality of the obtained PUFEM approximation, giving a first justification of the numerical treatment.

Consider the randomly excited Duffing oscillator:

$$m \ddot{X}(t; \theta) + b \dot{X}(t; \theta) + \eta_1 X(t; \theta) + \eta_3 X^3(t; \theta) = \Xi(t; \theta), \quad (6.1a)$$

$$X(t_0; \theta) = X^0(\theta), \quad \dot{X}(t_0; \theta) = \dot{X}^0(\theta). \quad (6.1b,c)$$

In equations (6.1), we assume  $b > 0$ ,  $\eta_1 < 0$  (bistable case), and  $\eta_3 > 0$ , to ensure global stability of the oscillator. The excitation is written in the form  $\Xi(t; \theta) = \xi_0 \tilde{\Xi}_0(t; \theta) + m_{\Xi}(t)$ , where the coefficient  $\xi_0$  has dimensions of force, leaving  $\tilde{\Xi}_0$  a dimensionless Gaussian excitation with zero-mean,  $m_{\Xi}(t) = 0$  and unitary variance  $\sigma_{\tilde{\Xi}_0}^2 = 1$ . In this way, the variance of the excitation  $\Xi$  is equal to  $\sigma_{\Xi}^2 = \xi_0^2$ .

Introducing the dimensionless variables

$$\tilde{t} = t \sqrt{\eta_1 / m}, \quad \tilde{X} = X \sqrt{\eta_3 / |\eta_1|}, \quad \tilde{X}_0 = X_0 \sqrt{\eta_3 / |\eta_1|} \quad \text{and} \quad \dot{\tilde{X}}_0 = \dot{X}_0 \sqrt{m \eta_3 / |\eta_1|},$$

equations (6.1a,b,c) take the following non-dimensional form:

$$\ddot{\tilde{X}}(\tilde{t}; \theta) + 2\zeta \dot{\tilde{X}}(\tilde{t}; \theta) - \tilde{X}(\tilde{t}; \theta) + \tilde{X}^3(\tilde{t}; \theta) = \tilde{\Xi}(\tilde{t}; \theta), \quad (6.2a)$$

$$\tilde{X}(t_0; \theta) = \tilde{X}_0(\theta), \quad \dot{\tilde{X}}(t_0; \theta) = \dot{\tilde{X}}_0(\theta), \quad (6.2b,c)$$

where  $\zeta = b / \left( 2\sqrt{m|\eta_1|} \right)$  is the dimensionless *damping ratio*,  $\tilde{\Xi}$  is the normalized excitation, expressed as

$$\tilde{\Xi}(\tilde{t}; \theta) = \Pi_{\Xi} \tilde{\Xi}_0(\tilde{t}; \theta) + m_{\Xi}(\tilde{t}), \quad m_{\Xi}(\tilde{t}) = (\eta_3 / |\eta_1|^3)^{1/2} m_{\Xi}(\tilde{t}), \quad (6.3a,b)$$

and  $\Pi_{\Xi} = \xi_0 \sqrt{\eta_3 / |\eta_1|^3}$  is the dimensionless *forcing coefficient*, which also plays the role of a *nonlinearity parameter*. Indeed, under the above choice of characteristic quantities, the effects of nonlinearity and the noise intensity are both included in the parameter  $\Pi_{\Xi}$  and studied jointly. Last, we specify  $\tilde{\Xi}_0(t; \theta)$  to be a Gaussian Filter (GF) excitation, with auto-covariance function

$$C_{\tilde{\Xi}_0 \tilde{\Xi}_0}(t, s) = C_{\tilde{\Xi}_0 \tilde{\Xi}_0}(t - s) = \exp\left(-a^2(t - s)^2\right) \cos(\omega_{\tilde{\Xi}_0}(t - s)), \quad (6.4)$$

where the parameter  $\omega_{\tilde{\Xi}_0}$  denotes the peak frequency of the excitation spectrum, and the parameter  $a$  calibrates the *correlation time of the excitation*,  $\tau_{cor}$ . The latter is defined in terms of the autocovariance function, [98] Chap. 2, Sec.9. In the present work we adopt the following definition of the correlation time

$$\tau_{cor} = C_{\Xi\Xi}^{-1}(0) \int_0^{+\infty} |C_{\Xi\Xi}(u)| du.$$

The autocovariance function of  $\tilde{\Xi}(\tilde{t}; \theta)$  takes the form  $C_{\tilde{\Xi}(\cdot)\tilde{\Xi}(\cdot)}(\tilde{t}, \tilde{s}) = \sigma_{\Xi}^2 C_{\tilde{\Xi}_0(\cdot)\tilde{\Xi}_0(\cdot)}(\tilde{t}, \tilde{s})$ , with variance  $\sigma_{\Xi}^2 = \Pi_{\Xi}^2$ .

Using the state-vector  $\mathbf{X} = (X_1, X_2) = (\tilde{X}, \dot{\tilde{X}})$ , the system of RDEs corresponding to equation (6.2a) takes the form of system (2.1) with  $N = 2$ . For this case, the functions  $h_{1,2}$ , in equation (2.1a), are specified as  $h_1(\mathbf{X}) = X_2$  and  $h_2(\mathbf{X}) = -X_1^3 + X_1 - 2\zeta X_2$ , while the excitation vector is  $\Xi = (0, \tilde{\Xi})$ . The Jacobian matrix of the vector  $\mathbf{h}$ , takes the form

$$\mathbf{J}^h(\mathbf{X}(t; \theta)) = \begin{bmatrix} 0 & 1 \\ 1 - 3X_1^2(t, \theta) & -2\zeta \end{bmatrix}. \quad (6.5)$$

Both SCT and novel genFPKE, corresponding to the oscillator under study, take the form of the general equation (2.6), differing only by the structure of their diffusion coefficients  $\mathcal{D}_{v_n}^{X^0 \Xi(\cdot)}$  and  $\mathcal{D}_{v_n}^{\Xi(\cdot) \Xi(\cdot)}$ , given by equations (5.19a,b) and (4.23a,b), respectively. Assuming, for simplicity, that the initial value is uncorrelated to the excitation,  $\mathbf{C}_{X^0 \Xi(\cdot)} = \mathbf{0}$ , the diffusion coefficients  $\mathcal{D}_{v_n}^{X^0 \Xi(\cdot)}$  become zero. Further, the coefficients  $\mathcal{D}_{v_1}^{\Xi(\cdot) \Xi(\cdot)}$  are also zero, since  $\Xi_1 = 0$ , by definition. For both cases, the diffusion coefficients  $\mathcal{D}_{v_2}^{\Xi(\cdot) \Xi(\cdot)}$  are of the following integral form

$$\mathcal{D}_{v_2}^{\Xi(\cdot) \Xi(\cdot)}[f_{X(\cdot)}(\cdot); \mathbf{x}, t] = \int_{t_0}^t C_{\tilde{\Xi}(\cdot)\tilde{\Xi}(\cdot)}(t, s) \left\{ \begin{array}{l} D_{v_2}^{\text{ngFPK}}[f_{X(\cdot)}(\cdot); \mathbf{x}, t, s] \\ D_{v_2}^{\text{SCT}}(\mathbf{x}, t, s) \end{array} \right\} ds, \quad (6.6)$$

The components  $D_{\nu 2}^{\text{ngFPK}}$ , corresponding to the novel gFPKE, are given by the formulae

$$D_{12}^{\text{ngFPK}}(f_{X(\cdot)}(\cdot); \mathbf{x}, t, s) = \Phi_{12}[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s), \quad (6.7a)$$

$$\begin{aligned} D_{22}^{\text{ngFPK}}(f_{X(\cdot)}(\cdot); \mathbf{x}, t, s) &= \\ &= 3 \left( m_{X_1^2}(t) - x_1^2 \right) \Phi_{12}[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s) + \Phi_{22}[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s). \end{aligned} \quad (6.7b)$$

where the matrix

$$\mathbf{R}(t) := \mathbf{R}[f_{X(\cdot)}(\cdot), t] = \begin{bmatrix} 0 & 1 \\ 1 - 3 m_{X_1^2}(t) & -2\zeta \end{bmatrix}$$

is the expected value of  $\mathbf{J}^h(\mathbf{X}(t; \theta))$ , equation (6.5), and the function  $m_{X_1^2}(t)$  is given by

$$m_{X_1^2}(t) := m_{X_1^2}(f_{X(t)}(\cdot); t) = \mathbb{E}^\theta[X_1^2(t; \theta)]. \quad (6.8)$$

The components  $D_{\nu 2}^{\text{SCT}}$ , corresponding to the SCT genFPKE, are given by

$$D_{12}^{\text{SCT}}(\mathbf{x}, t, s) = (t - s), \quad D_{22}^{\text{SCT}}(\mathbf{x}, t, s) = 1 - 2\zeta(t - s). \quad (6.9a,b)$$

Concerning the computation of the novel genFPKE, note that the function  $m_{X_1^2}(t)$  is actually a moment of the unknown response, realizing the dependence of the matrix  $\mathbf{R}$  on the density  $f_{X(\cdot)}(\cdot)$ . This somewhat peculiar term (6.8) calls for a special numerical treatment since, at each time instant, depends on the unknown density at that time. This peculiarity is treated by an iterative scheme as follows: the current-time value  $m_{X_1^2}(t)$ , needed for the calculation of diffusion coefficients (6.6), is first estimated by extrapolation based on the three previous time steps (after the second step), and then improved by iterations at the current time. That is, for  $\varepsilon > 0$  and  $m_{X_1^2}^{(0)}(t) = m_{X_1^2}(t)$ ,

- i) Calculate  $\mathcal{D}_{\nu 2}^{\Xi(\cdot)\Xi(\cdot)}$  by using the (initially extrapolated)  $m_{X_1^2}^{(i)}(t)$  and obtain the PUFEM approximation  $f_{X(t)}^{(i)}(\mathbf{x})$ ,
- ii) Calculate  $m_{X_1^2}^{(i+1)}(t)$  from  $f_{X(t)}^{(i)}(\mathbf{x})$  and check  $d = |m_{X_1^2}^{(i+1)}(t) - m_{X_1^2}^{(i)}(t)| < \varepsilon$ ,
- iii.1) if  $d < \varepsilon$ , set  $m_{X_1^2}(t) = m_{X_1^2}^{(i)}(t)$ ,  $f_{X(t)}(\mathbf{x}) = f_{X(t)}^{(i)}(\mathbf{x})$ , and continue to the next time,
- iii.2) if  $d > \varepsilon$ , return to step i) replacing  $m_{X_1^2}^{(i)}(t)$  by  $m_{X_1^2}^{(i+1)}(t)$ .

Usually, one or two iterations suffice to achieve convergence. Last, the state-transition matrix  $\Phi[\mathbf{R}](t; s)$  is approximated via a Magnus expansion with two terms, namely

$$\Phi[\mathbf{R}](t;s) \approx \exp \left[ \int_s^t \mathbf{R}(u_1) du_1 + \frac{1}{2} \int_s^t \int_s^{u_1} [\mathbf{R}(u_1), \mathbf{R}(u_1)] du_2 du_1 \right],$$

and the resulting matrix exponential is computed via explicit closed form expressions, see [86].

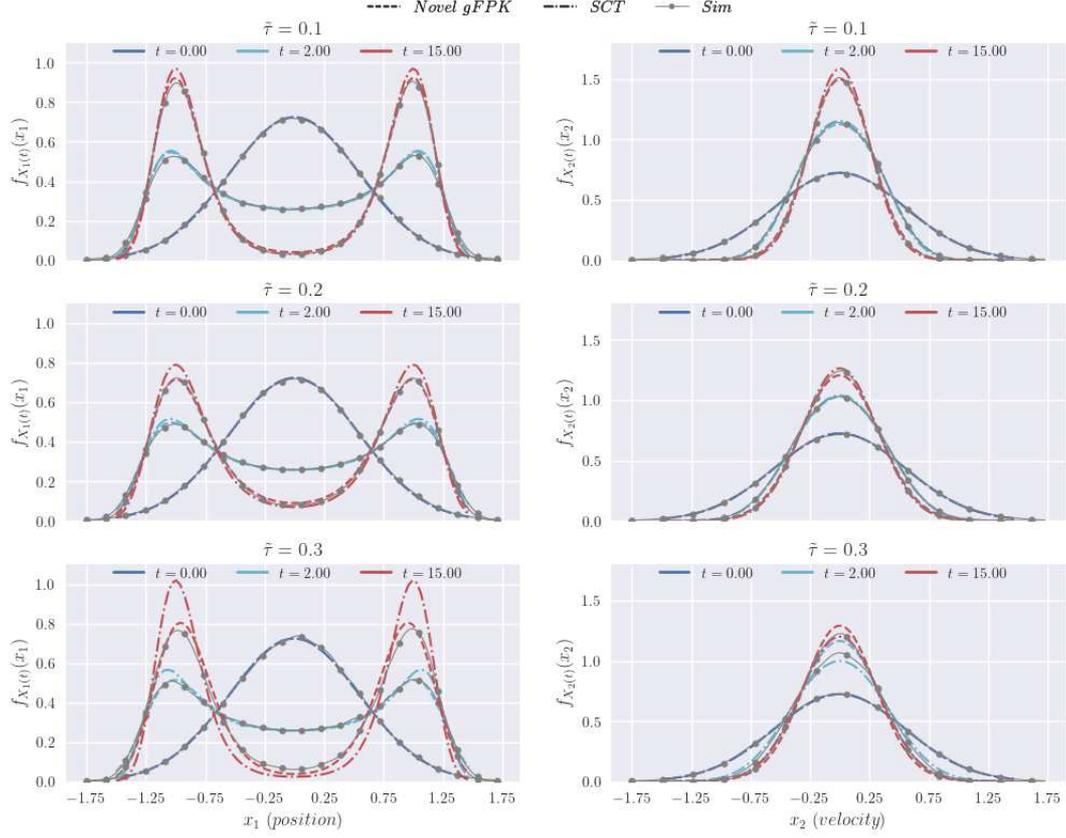
We consider the oscillator (6.1a) with dimensional parameters  $m = 1 \text{ kg}$ ,  $b = 1 \text{ kg sec}^{-1}$ ,  $\eta_1 = -1 \text{ kg sec}^{-2}$ ,  $\eta_3 = 0.36 \text{ kg m}^{-2} \text{ sec}^{-2}$  and  $\xi_0 = 1 \text{ kg m sec}^{-2}$ . This example corresponds to equation (6.2a) with  $\zeta = 0.5$ , subjected to a GF excitation  $\tilde{\Xi}(\tilde{t}; \theta)$  with intensity  $\Pi_{\Xi}^2 = 0.36$ . That is, we study a case with intermediate noise intensity or equivalently (for our normalization) an intermediately nonlinear one. Results are presented with respect to the normalized *correlation* time  $\tilde{\tau} = \tau_{cor} / \tau_{relax}$ , called relative correlation time, where  $\tau_{relax}$  denotes the relaxation time of the unforced harmonic oscillator. In all figures presented below, the final time is chosen to be in the long-time stationary regime, to check the validity of genFPKE in both the transient and the stationary regimes. The MC simulations are constructed from a sample of  $10^5$  numerical experiments for each tested case.

The numerical results presented below concern the non-dimensional oscillator (6.2a) with initial value and excitation parameter values given in Table 1 (Tilda is discarded from the notation).

**Table 1.** Numerical values of the parameters corresponding to the oscillator under numerical investigation in Figures 1 and 3.

<b>Oscillator / Excitation</b>					
parameters	$\zeta$	$m_{\Xi}$	$\sigma_{\Xi}^2 = \Pi_{\Xi}^2$	$\omega_{\Xi}$	$\tilde{\tau}$
values	0.5	0	0.36	2.5	[0.1, 0.2, 0.3]
<b>Initial Value</b>					
parameters	$\mathbf{m}_{X^0}$			$C_{X^0 X^0}$	
values	(0,0)			0.3 $\mathbf{I}$	

In Figure 3, we compare the 1D marginal distributions,  $f_{X_1(t)}(x_1)$  (position) and  $f_{X_2(t)}(x_2)$  (velocity), as obtained via the PUFEM solution of the SCT and novel genFPKE, as well as via MC simulation. In this test, we consider initial value and excitation of zero mean. We find that for  $\tilde{\tau} = 0.1$  both equations perform well enough, almost being in full agreement with MC simulations. However, as the relative correlation time  $\tilde{\tau}$  increases, SCT overestimates the peak values of the position density, especially in the steady state. This situation becomes more profound for  $\tilde{\tau} = 0.3$ . The pdf of the velocity,  $f_{X_2(t)}(x_2)$ , is well approximated by both equations.

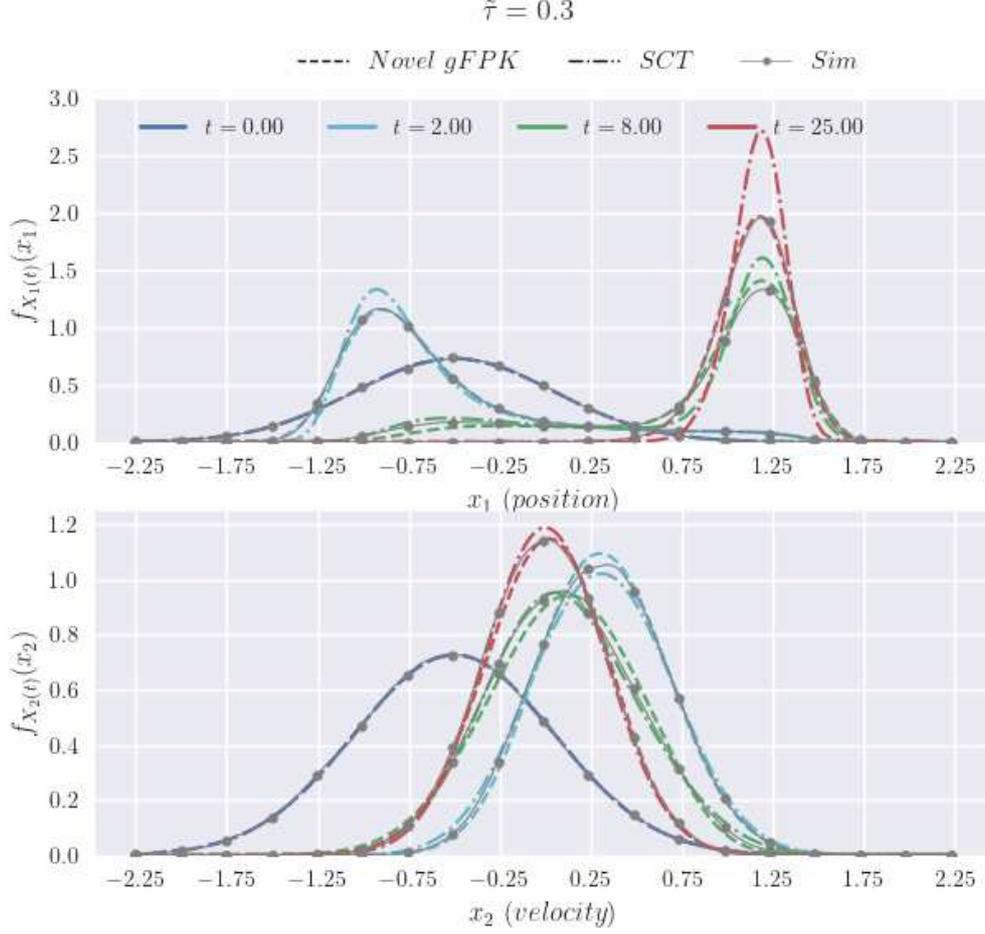


**Figure 3.** Evolution of response marginal pdfs for the oscillator (6.2a), configured as described in **Table 1**. Marginal pdfs obtained via the PUFEM solutions to the SCT genFPKE (dashed-dotted lines) and novel genFPKE (dashed lines) are compared to MC simulations (marked continuous lines) in different time instances. The greatest time corresponds to the long-time steady-state regime.

**Table 2.** Numerical values of the parameters corresponding to the oscillator under numerical investigation in Figures 3 and 4.

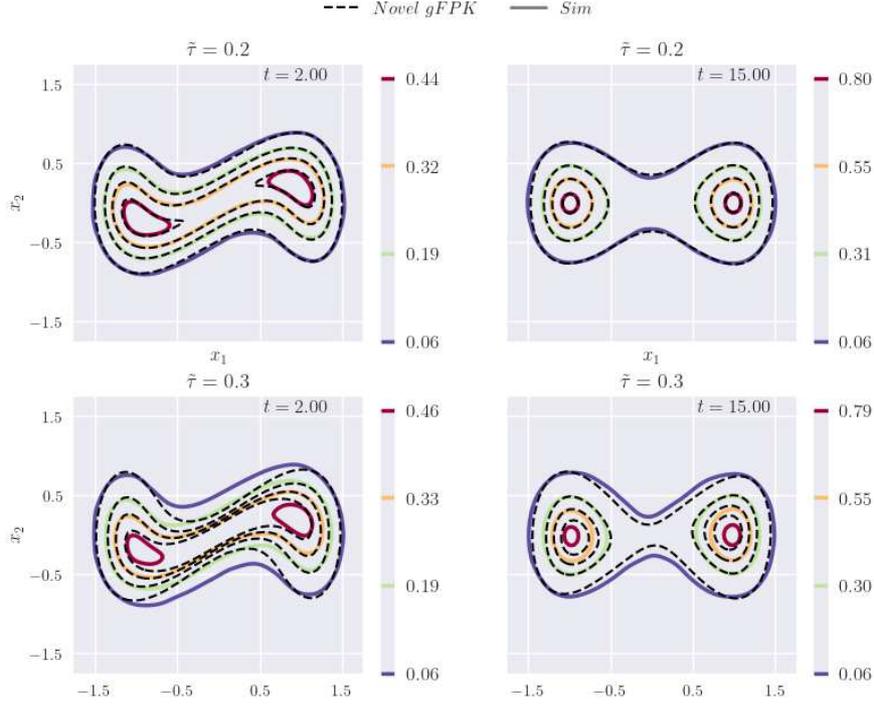
Oscillator / Excitation					
parameters	$\zeta$	$m_{\Xi}(t)$	$\sigma_{\Xi}^2 = \Pi_{\Xi}^2$	$\omega_{\Xi}$	$\tilde{\tau}$
values	0.5	$\frac{0.5 e^{6(t-1)}}{1+e^{6(t-1)}} \rightarrow 0.5$	0.36	2.5	0.3
Initial Value					
parameters	$m_{X^0}$			$C_{X^0 X^0}$	
values	$(-0.5, -0.5)$			$0.3 \mathbf{I}$	

In **Figure 4**, we demonstrate the marginal pdfs of the same oscillator but with initial value and excitation of non-zero mean as described in **Table 2**. The findings agree with the previous ones since, during the transition to the steady state, the SCT model results in an increasing overestimation of position's pdf, while the novel equation remains consistent with the MC simulations.

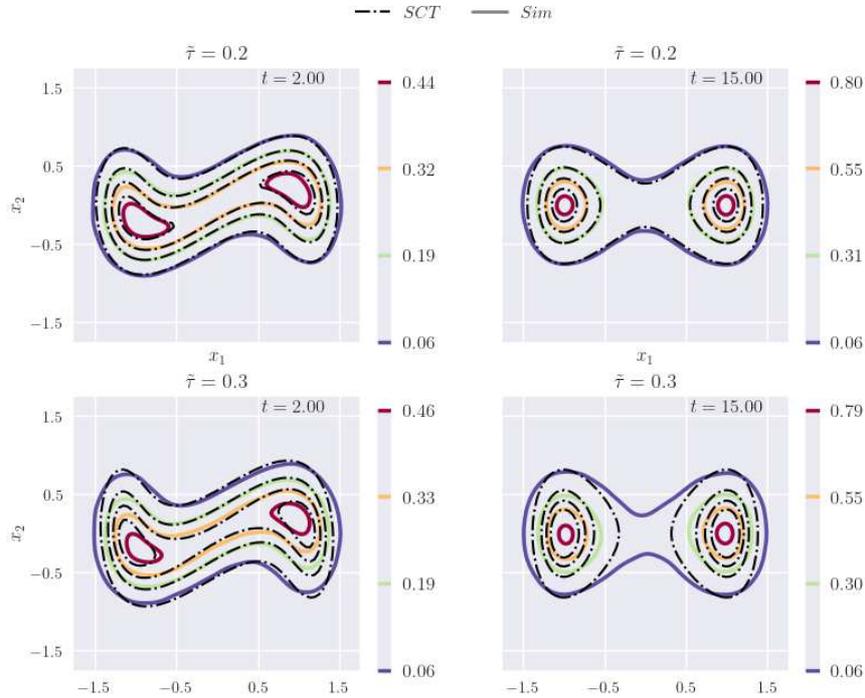


**Figure 4.** Evolution of response marginal pdfs for the oscillator (6.2a), configured as described in **Table 2**. Marginal pdfs obtained via the PUFEM solutions to the SCT genFPKE (dashed-dotted lines) and novel genFPKE (dashed lines) are compared to MC simulations (marked continuous lines) in different time instances. The greatest time corresponds to the long-time steady-state regime.

In Figure 5, we compare contour lines of the 2D response pdf for the same oscillator with parameter values given in **Table 1**, as obtained via PUFEM solution of the novel genFPKE, denoted  $f_{X(t)}^{n\text{gFPK}}(\mathbf{x})$ , with MC simulations. We observe that, for relative correlation time  $\tilde{\tau} = 0.3$ , in the steady state ( $t = 15$ ), the  $f_{X(t)}^{n\text{gFPK}}(\mathbf{x})$  contours are in good agreement with the MC simulations, except from the highest-level curve close to the density's picks. For the same oscillator, in Figure 6, we conduct the same comparison but for contour lines of the 2D response pdf, as obtained via PUFEM solution of the SCT genFPKE, denoted  $f_{X(t)}^{SCT}(\mathbf{x})$ . We see that for relative correlation time  $\tilde{\tau} = 0.3$ , the SCT genFPKE performs poorly at steady state ( $t = 15$ ), since the contours of  $f_{X(t)}^{SCT}(\mathbf{x})$  fails in capturing the geometric characteristics of the corresponding MC simulation. Further, it is worth noticing that the SCT genFPKE seems to perform better in the early transient state,  $t = 2$ , although its long-time steady state limit is a low-quality approximation, much worse than the one obtained by the novel genFPKE.

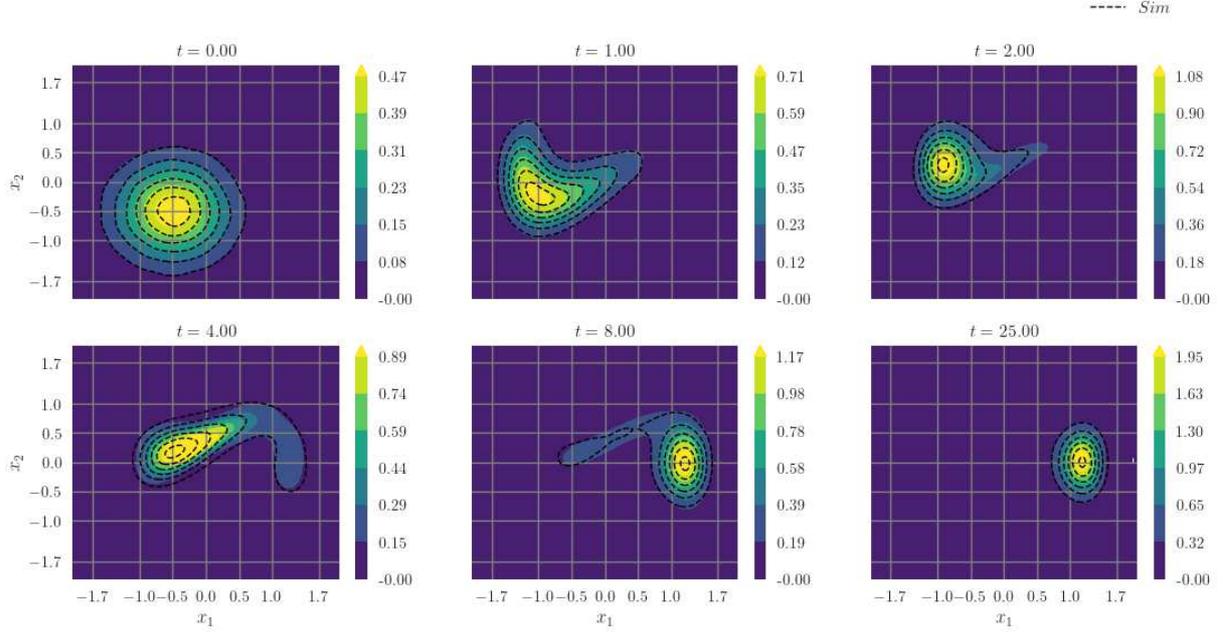


**Figure 5.** Contour lines of the 2D response pdf of the oscillator (6.2a), configured as described in **Table 1**. Contours of response pdfs  $f_{X(t)}^{n\text{ gFPK}}(\mathbf{x})$ , obtained via the PUFEM solutions of the novel genFPKE (dashed lines) are compared to MC simulations (colored continuous lines). Colors correspond to different level sets.



**Figure 6.** Contour lines of the 2D response pdf of the oscillator (6.2a), configured as described in **Table 1**. Contours of response pdfs  $f_{X(t)}^{SCT}(\mathbf{x})$ , obtained via the PUFEM solutions of the SCT genFPKE (dashed-dotted lines) are compared to MC simulations (colored continuous lines). Colors correspond to different level sets.

With the above results establishing that, for increasing correlation time, the novel genFPKE is a more appropriate model for the steady state response pdf, in **Figure 7**, we demonstrate the evolution of the 2D response pdf of the oscillator described by **Table 2**. Contour plots obtained via the solution of the novel genFPKE are compared with MC simulations.



**Figure 7.** Contour plots of the 2D response pdf of the oscillator (6.2a), configured as described in **Table 2**. Response pdfs  $f_{X(t)}^{n\text{genFPK}}(\mathbf{x})$ , obtained via the PUFEM solutions of the novel genFPKE are demonstrated in different time instances. Contour lines of corresponding MC simulations are denoted with black dashed-dotted lines.

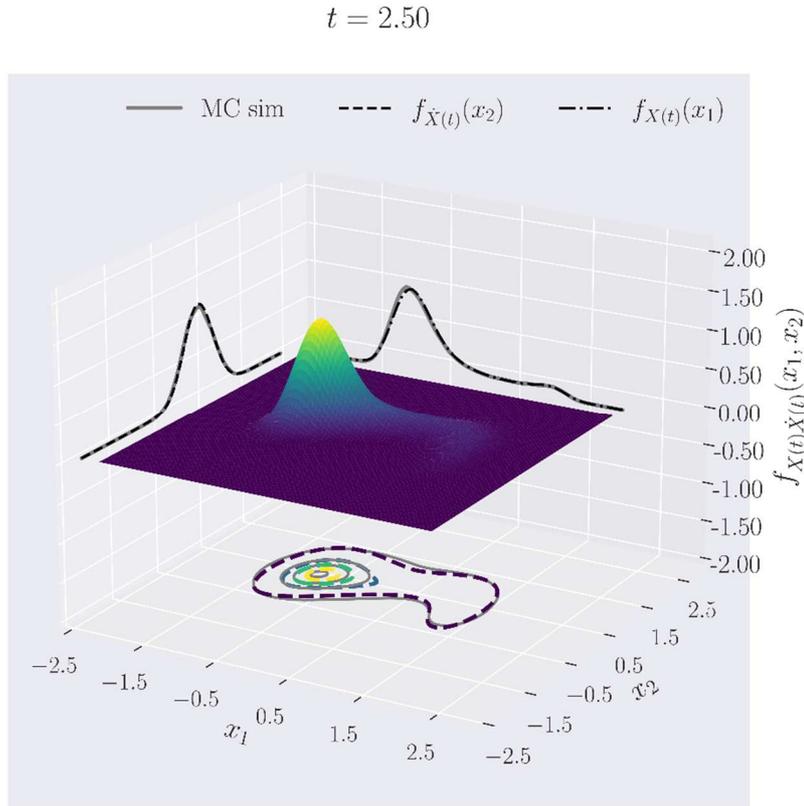
Last, in Figure 8 (Multimedia available online), we demonstrate the evolution of the response 1D marginal pdfs, 2D pdf and its contours, as obtained via PUFEM solution of the novel genFPKE, for the oscillator of **Table 2**, all compared to MC simulations. The video extends from the initial state, up to steady state, with a duration of 15 seconds.

## 7. Discussion and conclusions

In the present work, we presented derivations of pdf-evolution equations, governing the first-order response pdf of nonlinear systems of RDE under additive, colored Gaussian excitation. The derivation generalizes to the multidimensional case the ideas and techniques introduced in [25, 34] for the scalar analog. It is based on the SLE transformed by means of an extended version of the NF theorem, and the analytic calculation of the functional derivatives of the response with respect to initial values and excitation. Before applying the current-time closure, we separate the instantaneous mean value of the response from its random fluctuations, keeping the former intact in the final equation. This imitates the *Hänggi ansatz*, introduced in the 1D case by Hänggi *et al* in 1985 [20]. See also [22], 1995, pp. 271-273, where the same concept is discussed under the name *decoupling approximation*. Further, it renders the final pdf-evolution equation nonlinear and non-local in time, two features reflecting the non-Markovian character of the response.

The general equation (2.6) obtained herein can be used to derive simpler model equations, as e.g. the SCT genFPKE (4.22). Note that the latter is implicitly contained in various previous works dealing with the multiplicative excitation [44, 47, 91], although not stated explicitly for the case of additive excitation. In our approach the excitation is not limited to the Ornstein-Uhlenbeck process or any other prescribed correlation structure. Any colored Gaussian process can be considered as excitation. Also, any transient evolution of the excitation can be taken into account. Both the novel pdf-evolution equation (2.6) and the SCT genFPKE (4.22) have been tested numerically, for the case of an underdamped bistable Duffing oscillator under a Gaussian filter excitation, against MC simulations, showcasing good agreement, with overperformance of the novel equation (2.6) as the correlation time increases.

The systematic nature of the derivation procedure permits one to obtain better pdf-evolution equations by improving the approximations. For example, one can use a second-order current-time approximation and/or additional terms in the Magnus expansion to obtain improved equations. What is more important, the present approach can be generalized to the case of multiplicative excitation, covering a broader range of applications. The authors intend to address these extensions in future works.



**Figure 8.** Oscillator (6.2a), configured as described in **Table 2**. Evolution of response 1D marginal densities,  $f_{X_1(t)}(x_1)$  (dashed black line),  $f_{X_2(t)}(x_2)$  (dashed-dotted black line), 2D density  $f_{X(t)}^{n\text{ gFPK}}(\mathbf{x})$  (surface plot) and its contours (dashed colored lines), as obtained via PUFEM solution of the novel genFPKE, compared to MC simulations (solid grey line). (Multimedia available online)

## Appendix A: *List of Abbreviations* (in alphabetical order)

FF $\ell$  : Function Functional  
FPKE: Fokker-Plank-Kolmogorov Equation  
genFPKE: generalized FPKE  
GF: Gaussian Filter  
IVP(s): Initial Value Problem(s)  
MC: Monte Carlo  
NF: Novikov-Furutsu  
ODE(s): Ordinary Differential Equation(s)  
PDE(s): Partial Differential Equation(s)  
pdf(s): probability density function(s)  
PUFEM: Partition of Unity Finite Element Method  
RDE(s): Random Differential Equation(s)  
SCT: Small Correlation Time  
SLE: Stochastic Liouville Equation

## Appendix B: *On the state-transition matrix and its approximations*

Explicit forms of the state-transition matrix of a general (time-varying) linear system are provided by the Peano [81, 99, 100] and Magnus [83, 84] series expansions. We present herewith the standard formulation of both expansions, to fix the notation and facilitate the reader to follow the flow of calculations in Sec. 4 and 5.

Consider the linear, *time-varying* IVP

$$\dot{\mathbf{y}}(t) = \mathbf{A}(t) \mathbf{y}(t), \quad \mathbf{y}(t_0) = \mathbf{y}^0, \quad t \in [t_0, T]. \quad (\text{B1})$$

The corresponding *state-transition* matrix  $\Phi(t; t_0)$  realizes the solution of (B1) in the form  $\mathbf{y}(t) = \Phi(t; t_0) \mathbf{y}^0$  ( $\Phi(t_0; t_0) = \mathbf{I}$ ). In fact, for any given state  $\mathbf{y}(s)$ ,  $s \in [t_0, T]$ , it holds that  $\mathbf{y}(t) = \Phi(t; s) \mathbf{y}(s)$ ,  $\forall t \geq s$ . Further, a state-transition matrix is never singular, and it is  $C^{k+1}$  when  $\mathbf{A}(t)$  is  $C^k$ . Besides  $\Phi^{-1}(t; s) = \Phi(s; t)$ ,  $\forall s \in [t_0, T]$ , and  $\Phi(t; s)$  satisfies the *matrix differential equation*,  $\dot{\Phi}(t; s) = \mathbf{A}(t) \Phi(t; s)$ , with initial value  $\Phi(s; s) = \mathbf{I}$ . Given the fundamental matrix  $\mathbf{U}$  of (B1),  $\Phi$  is explicitly constructed as  $\Phi(t; s) = \mathbf{U}(t) \mathbf{U}^{-1}(s)$ . In some cases, we are obliged to consider simultaneously the state-transition matrices of two different linear time-varying systems (see, e.g., section 5.2). Then, use is made of the more complicated notation  $\Phi[\mathbf{A}](t; s)$ , where  $\mathbf{A}$  is the system matrix.

For a general time-varying linear system, the state-transition matrix  $\Phi(t; s)$  cannot be expressed in closed form. There are, however, series expansions of  $\Phi(t; s)$ , in terms of the *system matrix*  $A(t)$ . One such series expansion is the Peano-Baker series, obtained directly from Picard iterations, which has the form

$$\begin{aligned} \Phi(t; s) = \Phi[A](t; s) = I + \int_s^t A(u) du + \int_s^t A(u_1) \int_s^{u_1} A(u_2) du_2 du_1 + \\ + \int_s^t A(u_1) \int_s^{u_1} A(u_2) \int_s^{u_2} A(u_3) du_3 du_2 du_1 + \dots \end{aligned} \quad (\text{B2})$$

This series is uniformly convergent, see [81] Sec. 3, under the assumption of continuous  $A$ ; see also [101] Sec. 2.11 and [100]. In classical statistical mechanics, the above formula is usually identified as the definition of the ordered exponential, also expressed by the notation

$$\exp_{\text{ord}} \left( \int_s^t A(u) du \right) = I + \sum_{n=1}^{+\infty} \frac{1}{n!} \int_s^t \dots \int_s^t O[A(u_1) \dots A(u_n)] du_n \dots du_1,$$

where the operator  $O[\bullet]$  ensures the time ordering. In connection to the derivation of genFPKE, the ordered exponential is the central mathematical entity of the ordered cumulant expansion approach, see Sec. 1.2 for references. The series (B2) is closely related to the Dyson series used in quantum mechanics, [102] Sec. X.12, whose terms formally differs from the corresponding ones in Peano-Baker series by a factor  $(-i)^n$ . An alternative to the Peano-Baker series is the Magnus series expansion. The latter originate in the monumental work of Magnus [84] who followed the approach of expressing the solution of the non-autonomous matrix differential equation  $\dot{Y}(t) = A(t) Y(t)$ ,  $Y(s) = I$  as a matrix exponential

$$Y(t) = \Phi[A](t; s) Y(s) = \exp(\Omega(t; s)). \quad (\text{B3})$$

Then, the matrix  $\Omega(t; s)$  is expressed via the series

$$\Omega(t; s) := \sum_{i=1}^{+\infty} \Omega_i(t; s), \quad (\text{B4})$$

where, by denoting  $[A, B] = AB - BA$  the matrix commutator, its first three terms read

$$\begin{aligned} \Omega_1(t; s) &= \int_s^t A(u) du, & \Omega_2(t; s) &= \frac{1}{2} \int_s^t \int_s^{u_1} [A(u_1), A(u_2)] du_2 du_1, \\ \Omega_3(t; s) &= \frac{1}{6} \int_s^t \int_s^{u_1} \int_s^{u_2} [A(u_1), [A(u_2), A(u_3)]] + [A(u_3), [A(u_2), A(u_1)]] du_3 du_2 du_1. \end{aligned}$$

In general, the Magnus expansion is a handy tool in many situations, since it directly provides an exponential representation of the state-transition matrix. Conditions under which (B3) exists are discussed in [83] Sec. 2.7.1, and the convergence of the series (B4) has been extensively studied by many authors, see [103], [83] Sec. 2.7.2 and references therein. Despite that

the Magnus expansion usually has a small radius of convergence, it is a precious tool for approximations in small time intervals  $t - s$ , since it is well behaved under truncation of any order, maintaining qualitative and often geometric characteristics of the solution, see [83] Sec. 1.1. These features make Magnus expansion a more suitable tool, both for analytic and numerical approximations, even though it may seem easier to perform calculations/computations with the formally simpler Peano-Baker series. Both above representations of  $\Phi$  are utilized in Sections 4 and 5, respectively.

Last, it is worth mentioning that there are two special cases for which the series (B2) can be summed, obtaining a closed-form expression for  $\Phi$ . The first is for constant  $A$  (time-invariant systems), and the second is the case where  $A(\tau)$  commutes with its integral (special time-varying structure) [81, Section 1.5]. In these cases,  $\Phi$  attains the form of the matrix exponential  $\Phi = \exp(\int_{t_0}^t A(\tau) d\tau)$ . In the above cases, all commutators in the Magnus series (B4) become zero.

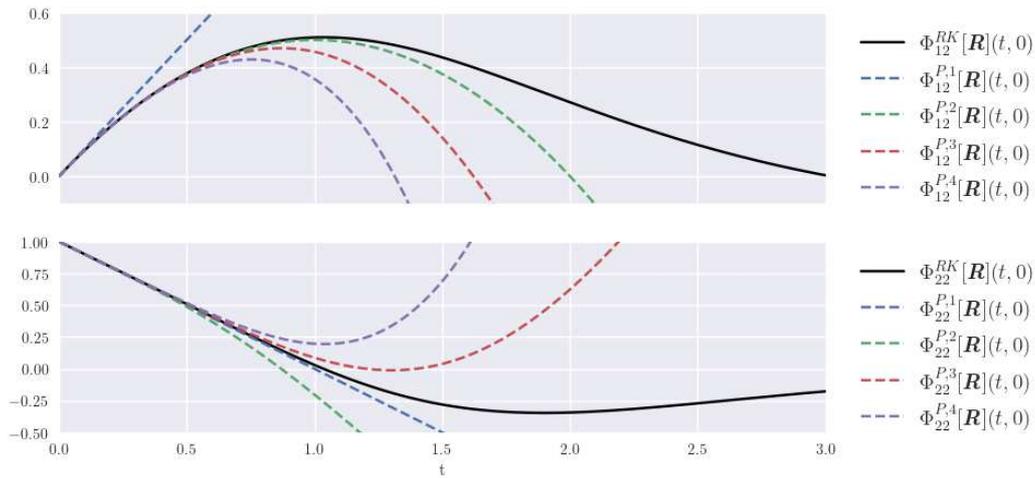
We close this Appendix by constructing an example to compare the efficiency of the Peano-Baker and Magnus expansions. The example is motivated from Sec. 6, where we solve the novel genFPKE (2.6), corresponding to the Duffing oscillator (6.2a). In this case, the Magnus expansion is used for the determination of the components  $\Phi_{12}$  and  $\Phi_{22}$ , of the state-transition matrix  $\Phi[\mathbf{R}[f_{X(\cdot)}(\cdot), \cdot]](t; s)$ , required for the computation of the diffusion coefficients (6.6) Sec. 6. The matrix  $\mathbf{R}(t) := \mathbf{R}[f_{X(\cdot)}(\cdot), t]$  has the form

$$\mathbf{R}(t) = \begin{bmatrix} 0 & 1 \\ 1 - 3 m_{X_1^2}(t) & -2\zeta \end{bmatrix},$$

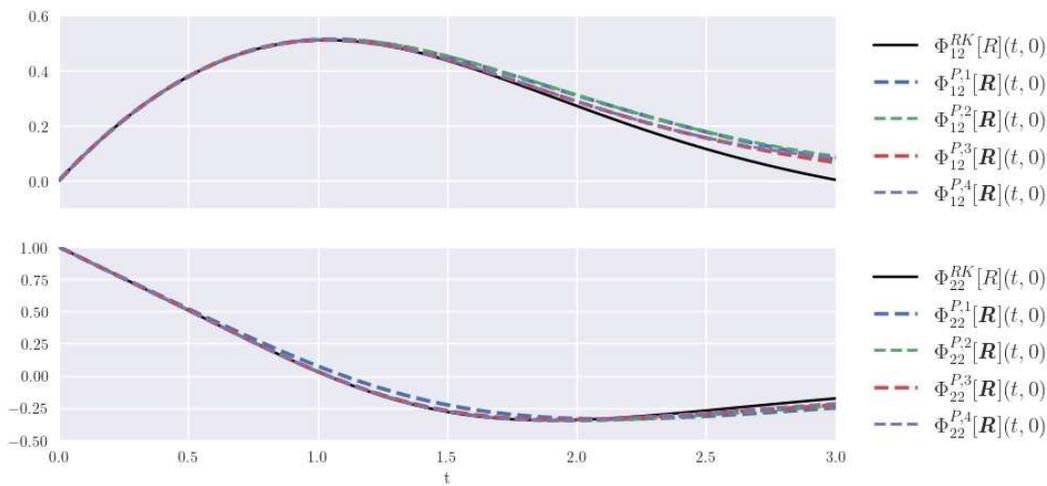
where the second moment  $m_{X_1^2}(t)$  is unknown since it depends on the unknown density  $f_{X(t)}(\mathbf{x})$ . However, for a specific oscillator (i.e. oscillator (6.2a), with parameter values as in Table 2), we can retrieve  $m_{X_1^2}(t)$  from the data of the MC simulation, making the matrix  $\mathbf{R}$  a priori known for a given time interval  $[s, T]$ . Then, the state-transition matrix  $\Phi[\mathbf{R}](t; s)$  is computed by solving the IVPs

$$\dot{\mathbf{y}}_i(t) = \mathbf{R}(t) \mathbf{y}_i(t), \quad \mathbf{y}_i(s) = \mathbf{e}_i, \quad i = 1, 2,$$

via a fourth order Runge-Kutta (RK) method. That is, we approximate  $\Phi[\mathbf{R}](t; s)$  via  $\Phi^{RK}[\mathbf{R}](t; s) = (\mathbf{y}_1(t), \mathbf{y}_2(t))$  ( $\mathbf{y}_{1,2}$  are column vectors), which is considered as reference solution. In Figures B1 and B2, we compare the RK solution  $\Phi_{i2}^{RK}[\mathbf{R}](t; s)$ ,  $i = 1, 2$ , with the Peano-Baker approximation  $\Phi_{i2}^{P,n}[\mathbf{R}](t; s)$ , obtained via the truncated series (B2) with  $n = 1, 2, 3, 4$  terms, and the Magnus approximation  $\Phi_{i2}^{M,n}[\mathbf{R}](t; s)$ , obtained via the exponentiation of the truncated series (B4) with  $n = 1, 2, 3, 4$  terms.



**Figure B5.** Comparison of Peano Baker approximation  $\Phi_{i2}^{P,n}[\mathbf{R}](t; s=0)$  (dashed lines) and RK solution (continuous lines).



**Figure B6.** Comparison of Magnus approximation  $\Phi_{i2}^{M,n}[\mathbf{R}](t; s=0)$  (dashed lines) and RK solution (continuous lines).

The superiority of the Magnus approximation over the Peano approximation along the full range  $[0, T=3]$  is clearly seen in the above example. This behavior has been observed in many other examples we have investigated numerically.

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## Supplementary Material

to

### A systematic path to non-Markovian dynamics II: Probabilistic response of nonlinear multidimensional systems to Gaussian colored noise excitation

#### On the underdamped linear oscillator and corresponding numerical results

In continuation of Section 4.1.1 of the main paper, here we consider an underdamped ( $\zeta < 1$ ) linear oscillator, equation (4.8) of the main paper. The state-space representation  $\mathbf{X}^T = (X_1, X_2)$  of equation (4.8), results in the following system of linear RDEs, see equations (4.9a,b) and (2.1a,b),

$$\dot{\mathbf{X}}(t; \theta) = \begin{bmatrix} 0 & 1 \\ -\omega_0^2 & -2\zeta\omega_0 \end{bmatrix} \mathbf{X}(t; \theta) + \boldsymbol{\Xi}(t; \theta), \quad (1a)$$

$$\mathbf{X}(t_0; \theta) = (X_1^0(\theta), X_2^0(\theta)), \quad (1b)$$

where the excitation vector reads as  $\boldsymbol{\Xi}(t; \theta) = (0, \Xi(t; \theta))^T$ , and its component  $\Xi_2 = \Xi$ , is considered a colored Gaussian excitation of non-zero mean,  $m_\Xi(t) \neq 0$ , in general. It is convenient to represent the random excitation in the form

$$\Xi(t; \theta) = \xi_0 \tilde{\Xi}(t; \theta) + m_\Xi(t), \quad (2)$$

where the coefficient  $\xi_0$  has dimensions  $m \text{ sec}^{-2}$ , since equation (4.8) is divided by mass, leaving  $\tilde{\Xi}$  a dimensionless excitation which exhibits a unitary variance  $\sigma_{\tilde{\Xi}}^2 = 1$ , and zero-mean,  $m_{\tilde{\Xi}}(t) = 0$ . In this way, equation (2) implies an autocorrelation function  $C_{\Xi\Xi}(t, s) = \sigma_\Xi^2 C_{\tilde{\Xi}\tilde{\Xi}}(t, s)$ , with variance  $\sigma_\Xi^2 = \xi_0^2$ . Further, we assume a stationary Gaussian Filter (GF) excitation with autocovariance function

$$C_{\Xi\Xi}(t, s) = C_{\tilde{\Xi}\tilde{\Xi}}(t-s) = \exp(-a^2(t-s)^2) \cos(\omega_\Xi(t-s)),$$

where  $\omega_\Xi$  denotes the central frequency of excitation's spectrum, and  $a$  is a shape parameter controlling the *correlation time of the excitation*. The latter is denoted by  $\tau_{cor}$ , and is defined via the autocovariance function, by the equation  $\tau_{cor} = C_{\Xi\Xi}^{-1}(0) \int_0^{+\infty} |C_{\Xi\Xi}(u)| du$ .

The governing pdf-evolution equation is  $\partial f_{\mathbf{X}(t)}(\mathbf{x}) / \partial t + L[f_{\mathbf{X}(t)}(\mathbf{x})] = 0$ , where the second-order partial differential operator  $L$  is given by equation (4.13) and is repeated here for convenience.

$$\begin{aligned} L[\cdot] = & -U^{(1)}(t; t_0) \partial_{x_2 x_1} \cdot - U^{(2)}(t; t_0) \partial_{x_2 x_2} \cdot + \\ & + x_2 \partial_{x_1} \cdot + \left( m_{\Xi(\cdot)}(t) - \omega_0^2 x_1 - 2\zeta\omega_0 x_2 \right) \partial_{x_2} \cdot - 2\zeta\omega_0 \cdot. \end{aligned}$$

Now, for the present case, we determine the functions  $U^{(\nu)}(t; t_0)$ , equations (4.12a,b), which are sums of the diffusion coefficients  $\mathcal{D}_{\nu 2}^{X^0 \Xi(\cdot)}$  and  $\mathcal{D}_{\nu 2}^{\Xi(\cdot) \Xi(\cdot)}(t)$ , see equation (4.11). Assuming for simplicity, that the excitation  $\Xi(t; \theta)$  is uncorrelated to the initial value  $X^0(\theta)$ , we have that  $\mathbf{C}_{X^0 \Xi(\cdot)} = \mathbf{0}$ , and the diffusion coefficients  $\mathcal{D}_{\nu 2}^{X^0 \Xi(\cdot)}$  become zero. Then, via equations (4.12a,b), we obtain

$$U^{(\nu)}(t; t_0) = \mathcal{D}_{\nu 2}^{\Xi(\cdot) \Xi(\cdot)}(t) = \int_{t_0}^t C_{\Xi(\cdot) \Xi(\cdot)}(t, s) \Phi_{\nu 2}^{\Xi}(t, s) ds,$$

where the components of the state-transition matrix,  $\Phi_{\nu 2}^{\Xi}(t, s)$ , are given by equation (4.10). By setting  $a = -\zeta \omega_0$  and  $b = \omega_0(1 - \zeta^2)^{1/2}$ , and substituting the components of the state-transition matrix, we obtain

$$U^{(1)}(t; t_0) = \frac{1}{\gamma} \int_{t_0}^t C_{\Xi(\cdot) \Xi(\cdot)}(t, s) e^{-a(t-s)} \sin(\gamma(t-s)) ds,$$

$$U^{(2)}(t; t_0) = \frac{1}{\gamma} \int_{t_0}^t C_{\Xi(\cdot) \Xi(\cdot)}(t, s) e^{-a(t-s)} (a \sin(\gamma(t-s)) - \gamma \cos(\gamma(t-s))) ds,$$

The above completely determines the corresponding genFPKE of the linear system of RDEs (1). In this linear case, the analytic solution of the corresponding genFPKE is available. It is the bivariate Gaussian density with *mean value* vector

$$\mathbf{m}_X(t) = \Phi^{X^0}(t, t_0) \mathbf{m}_{X^0} + \int_{t_0}^t \Phi^{\Xi}(t, s) \mathbf{m}_{\Xi}(s) ds,$$

and *autocovariance* matrix

$$\begin{aligned} \mathbf{C}_{XX}(t) &= \mathbb{E}^\theta \left[ \left( X(t, \theta) X^\top(t, \theta) \right) \right] - \mathbf{m}_X(t) \mathbf{m}_X^\top(t) = \\ &= \Phi^{X^0}(t, t_0) \mathbf{C}_{X^0 X^0} \left( \Phi^{X^0}(t, t_0) \right)^\top + \int_{t_0}^t \int_{t_0}^t \Phi^{\Xi}(t, s_1) \mathbf{C}_{\Xi \Xi}(s_1, s) \left( \Phi^{\Xi}(t, s) \right)^\top ds_1 ds, \end{aligned}$$

where the matrix  $\Phi^{\Xi}$  is given by equation (4.10), and the matrix  $\Phi^{X^0}$  results by substituting  $s = t_0$  in the latter.

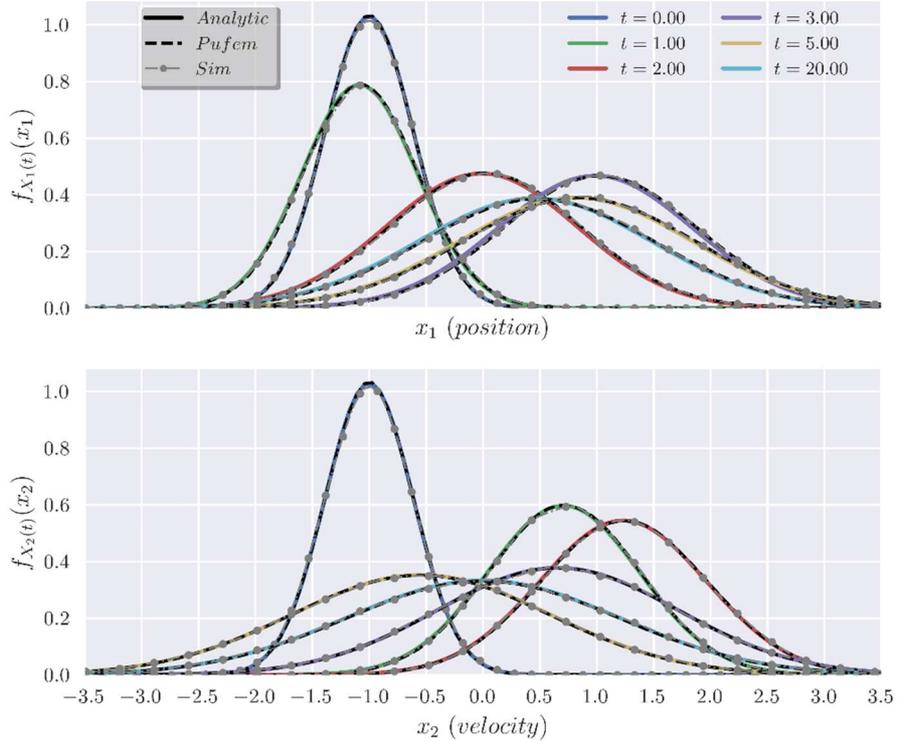
**Remark 1.** The pdf-evolution equation for a linear damped oscillator is both trivial and interesting. It is trivial since we know its solution in closed form; and it is interesting since we can use it as a benchmark problem to check the sufficiency of the Monte Carlo simulations, as well as *some* features of the numerical solution scheme developed for solving the general equation (2.6); see Section 2.2 and 5.2.

The numerical results to be presented subsequently concern the oscillator (1) with parameter values given in Table 1. In all figures presented below, the largest time for which results are shown is chosen to be well-within the long-time stationary regime, in order to check the va-

lidity of genFPKE in both the transient and the stationary regimes. The presented MC simulations are constructed from a sample of  $10^5$  numerical experiments. In **Figure 1**, the marginal pdfs of the response are demonstrated in different time instances. In **Figure 2**, the 2D response pdf is demonstrated at different times. In both figures, PUFEM approximations of the densities are compared with analytic ones and MC simulations.

**Table 1.** Configuration of the problem under numerical investigation.

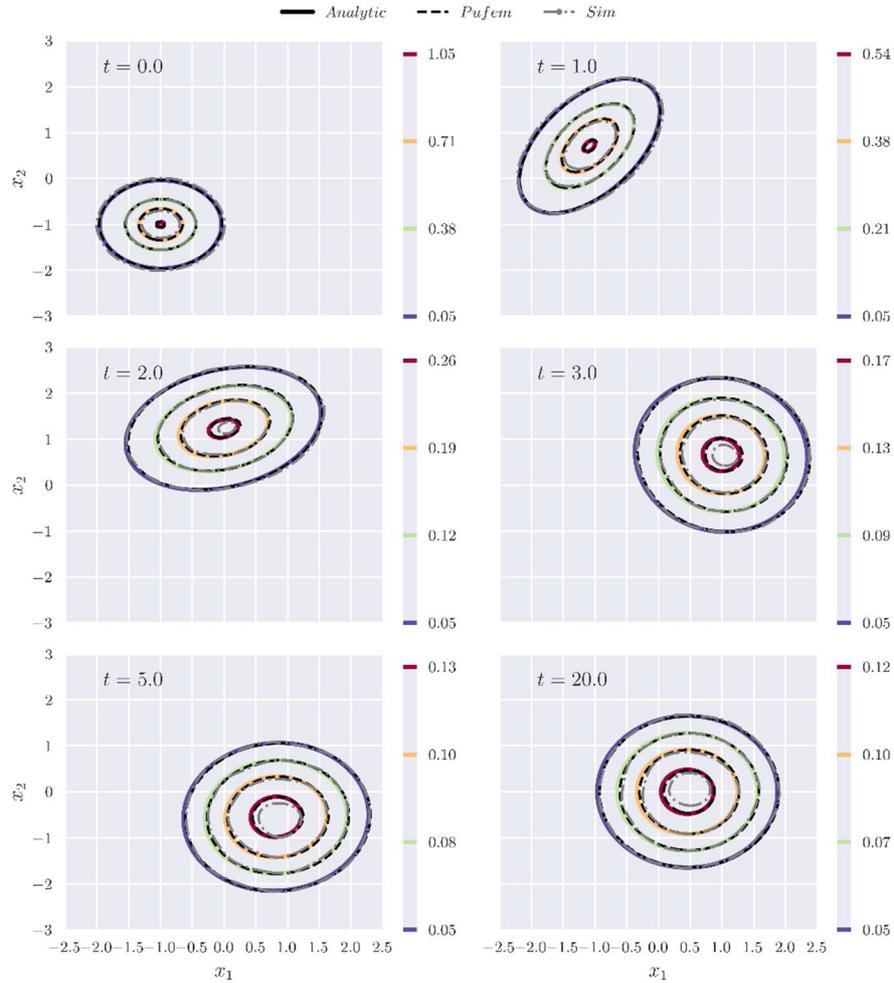
Oscillator				
parameters	$\zeta$		$\omega_0$	
values	0.25		1 sec <sup>-1</sup>	
Initial Value				
parameters	$m_{x^0}$		$C_{xx}$	
values	$(-1m, -1m \text{ sec}^{-1})$		0.15 I m <sup>2</sup> sec <sup>-2</sup>	
Excitation				
parameters	$m_{\Xi}$	$\sigma_{\Xi}^2$	$\omega_{\Xi}$	$\tau_{corr}$
values	0.5 m sec <sup>-1</sup>	1 m sec <sup>-2</sup>	1.5 sec <sup>-1</sup>	2 sec



**Figure 1.** Evolution of response marginal pdfs for the oscillator (1) configured as described in Table 1. Analytic marginal pdfs (continuous colored lines) are compared to corresponding obtained via the PUFEM solution of the gen FPKE (dashed black lines) and MC simulation (marked grey lines), at different times.

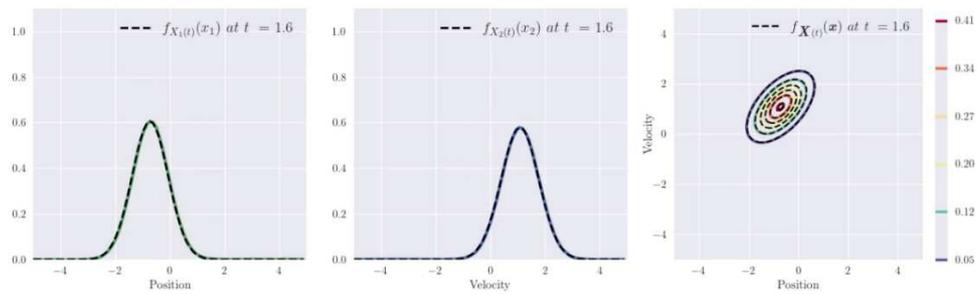
The results suggest that the PUFEM approximation, as well as the MC simulation are in good agreement with the analytical solution of the linear genFPKE both in the transient and long

steady state, on the level of 1D (Figure 1) and 2D pdfs (Figure 2). Further, considering a case with constant non-zero mean excitation, we find that the long time,  $t > 15$ , mean value of the position  $X_1(t; \theta)$ , becomes equal to the excitation mean value,  $m_{X_1}(t) = \mathbb{E}^\theta [X_1(t; \theta)] \xrightarrow{t \rightarrow +\infty} m_{\Xi} = 0.5$ , as expected.



**Figure 2.** Evolution contours of 2D response pdf for the for the oscillator (1) configured as described in Table. 1. Contour lines of the analytic pdf (continuous colored lines) are compared to corresponding PUFEM approximations (dashed black lines) and MC simulation (dashed dotted grey lines), at different time instances.

In **Figure 3** (Multimedia available online), PUFEM approximations of the response 1D and 2D pdfs are compared with corresponding analytic densities.



**Figure 3.** Evolution of response pdfs for the linear RDE (1), configured as described in Table. 1. In left and middle panel, analytic marginal pdfs (continuous colored lines) are compared to PUFEM approximations (dashed black lines). In the right panel, the 2D pdf is demonstrated. Contour lines of the analytic pdf (continuous colored lines) are compared to corresponding PUFEM approximations (dashed black lines). (Multimedia available online)