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Direct quadrature method of moments solution of the Fokker–Planck equation

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Abstract

The direct quadrature method of moments is presented as an efficient and accurate means of numerically computing solutions of the Fokker–Planck equation corresponding to stochastic nonlinear dynamical systems. The theoretical details of the solution procedure are first presented. The method is then used to solve Fokker–Planck equations for both 1D and 2D (noisy van der Pol oscillator) processes which possess nonlinear stochastic differential equations. Higher-order moments of the stationary solutions are computed and prove to be very accurate when compared to analytic (1D process) and Monte Carlo (2D process) solutions.

1. Introduction

Characterization of the response of stochastic systems is of interest for engineers in many different disciplines. This is particularly true in the field of structural dynamics where loads can often be thought of as random processes. For example in the field of aeroelasticity, Ibrahim and his colleagues considered the pressure fluctuations due to a turbulent boundary layer as random forces when analyzing panel flutter [1–3]. The response of a structural dynamic system to random excitation having delta-correlation can be considered a Markov process. The transition probability density of such a system is governed by an appropriate Fokker–Planck equation.

Exact solutions of the Fokker–Planck equation are known for only a few systems. In most cases, approximate solutions need to be found using either analytic or numerical methods. The text by Risken [4] presents many such analytical methods. Examples of approximate analytical solutions are the van Kampen expansion method [5,6], the method of matrix continued fractions [7] and path integral solutions [8]. In terms of numerical methods, finite difference and finite element methods appear to be the most popular [9–12]. While these methods can give accurate solutions, the computational expense can be prohibitive for Fokker–Planck equations with dimensions larger than two.

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In this paper we present an efficient and accurate method for the solution of the Fokker–Planck equation. This method is based upon the direct quadrature method of moments (DQMOM) first introduced by Fox and colleagues [13–15] for the numerical solution of the population balance equations for multi-phase flow predictions. Recently this method has also been used to compute numerical solutions for the Boltzmann equation [16]. Here DQMOM will be used to compute numerical solutions for 1D and 2D Fokker–Planck equations, and stationary moment results from these solutions are compared to results from analytical and numerical solutions.

2. Theory

Given the set of stochastic differential equations in N variables $\mathbf{x} = \{x_1, x_2, \ldots, x_N\}$:

$$\dot{x}_i = h_i(\mathbf{x}, t) + g_{ij}(\mathbf{x}, t)\Gamma_j(t), \tag{1}$$

where $\Gamma_j(t)$ are Gaussian random variables with the following correlations:

$$\langle \Gamma_i(t) \rangle = 0, \quad \langle \Gamma_i(t)\Gamma_j(t') \rangle = 2\delta_{ij}\delta(t - t'), \tag{2}$$

with δ_{ij} the Kronecker delta and $\delta(t - t')$ the delta function, a Fokker–Planck equation for the transition probability $P(\mathbf{x}, t|\mathbf{x}', t')$ can be written in the following form:

$$\frac{\partial P(\mathbf{x}, t|\mathbf{x}', t')}{\partial t} = -\frac{\partial}{\partial x_i}[D_i^{(1)}(\mathbf{x}, t)P(\mathbf{x}, t|\mathbf{x}', t')] + \frac{\partial^2}{\partial x_i\,\partial x_j}[D_{ij}^{(2)}(\mathbf{x}, t)P(\mathbf{x}, t|\mathbf{x}', t')]. \tag{3}$$

It can also be shown that the probability density function $f(\mathbf{x}, t)$ also satisfies the Fokker–Planck equation:

$$\frac{\partial f(\mathbf{x}, t)}{\partial t} = -\frac{\partial}{\partial x_i}[D_i^{(1)}(\mathbf{x}, t)f(\mathbf{x}, t)] + \frac{\partial^2}{\partial x_i\,\partial x_j}[D_{ij}^{(2)}(\mathbf{x}, t)f(\mathbf{x}, t)]. \tag{4}$$

In Eqs. (3) and (4) the drift ($D_i^{(1)}(\mathbf{x}, t)$) and diffusion ($D_{ij}^{(2)}(\mathbf{x}, t)$) coefficients are defined as (using the notation of Eq. (1))

$$D_i^{(1)}(\mathbf{x}, t) = h_i(\mathbf{x}, t), \tag{5}$$

$$D_{ij}^{(2)}(\mathbf{x}, t) = g_{ik}(\mathbf{x}, t)g_{jk}(\mathbf{x}, t) \tag{6}$$

and are derived using the Itô calculus [4]. Note in Eqs. (3) and (4) summation notation is assumed.

In order to simplify the derivations, Eq. (4) will be specialized to the problem of $N = 2$ and all cross-diffusion terms will be assumed to be zero ($D_{12}^{(2)} = D_{21}^{(2)} = 0$). Also $D_{11}^{(2)}$ will be assumed to be zero. In practice, generalizing the method (to be discussed in this paper) to higher dimensions with all terms included does not complicate the computational procedure. With the above simplifications we get the following for the Fokker–Planck equations:

$$\frac{\partial f(\mathbf{x}, t)}{\partial t} = -\frac{\partial}{\partial x}[D_1^{(1)}f(\mathbf{x}, t)] - \frac{\partial}{\partial y}[D_2^{(1)}f(\mathbf{x}, t)] + \frac{\partial^2}{\partial y^2}(D_{22}^{(2)}f(\mathbf{x}, t)), \tag{7}$$

where now $\mathbf{x} = \{x, y\}^{\mathrm{T}}$.

In the DQMOM approach the probability density is written as a weighted summation of products of Dirac delta functions:

$$f(\mathbf{x}, t) = \sum_{i=1}^{M} w_i(t)\delta(x - x_i(t))\delta(y - y_i(t)), \tag{8}$$

where M is the number of delta functions (compute nodes) and $w_i(t)$, $x_i(t)$ and $y_i(t)$ are the dependent variables for compute node i. In the rest of the paper w_i will be called weights and x_i, y_i the abscissas. Also the explicit expression of the dependent variables as functions of time will be dropped in order to condense the notation. If the delta functions $\delta(x - x_i)$ and $\delta(y - y_i)$ are written as $\delta_i^{(x)}$ and $\delta_i^{(y)}$, respectively, substitution of Eq. (8) into

Eq. (7) will result in the following:

$$\sum_{i=1}^{M}\left[\frac{\partial w_i}{\partial t}\delta_i^{(x)}\delta_i^{(y)} - w_i\frac{\partial x_i}{\partial t}\frac{\partial \delta_i^{(x)}}{\partial x}\delta_i^{(y)} - w_i\frac{\partial y_i}{\partial t}\delta_i^{(x)}\frac{\partial \delta_i^{(y)}}{\partial y}\right] = \sum_{i=1}^{M}\left[-\frac{\partial}{\partial x}(D_1^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}) - \frac{\partial}{\partial y}(D_2^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}) + \frac{\partial^2}{\partial y^2}(D_{22}^{(2)}w_i\delta_i^{(x)}\delta_i^{(y)})\right]. \quad (9)$$

Defining new variables, which we will call the weighted abscissas, $\mu_i^{(x)} = w_i x_i$ and $\mu_i^{(y)} = w_i y_i$, Eq. (9) becomes

$$\sum_{i=1}^{M}\left[\frac{\partial w_i}{\partial t}\delta_i^{(x)}\delta_i^{(y)} - x_i\frac{\partial \mu_i^{(x)}}{\partial t}\frac{\partial \delta_i^{(x)}}{\partial x}\delta_i^{(y)} + x_i\frac{\partial w_i}{\partial t}\frac{\partial \delta_i^{(x)}}{\partial x}\delta_i^{(y)} - \frac{\partial \mu_i^{(y)}}{\partial t}\frac{\partial \delta_i^{(y)}}{\partial y}\delta_i^{(x)} + y_i\frac{\partial w_i}{\partial t}\frac{\partial \delta_i^{(y)}}{\partial y}\delta_i^{(x)}\right] = \sum_{i=1}^{M}\left[-\frac{\partial}{\partial x}(D_1^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}) - \frac{\partial}{\partial y}(D_2^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}) + \frac{\partial^2}{\partial y^2}(D_{22}^{(2)}w_i\delta_i^{(x)}\delta_i^{(y)})\right]. \quad (10)$$

At this point we have one equation in $3M$ unknowns. In order to close this equation, we will take $3M$ moments of it. Recalling that the generalized moment $\langle x^r y^s\rangle$, for non-negative integers r and s, is given by the expression

$$\langle x^r y^s\rangle = \int_{-\infty}^{\infty} x^r y^s f(x,y,t)\,\mathrm{d}x\,\mathrm{d}y, \quad (11)$$

the evolution of $\langle x^r y^s\rangle$ can be obtained by taking the moment of Eq. (10) (after interchanging the order of summation and integration and combining the sums on the left- and right-hand sides):

$$\sum_{i=1}^{M}\left[\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} x^r y^s\left[\frac{\partial w_i}{\partial t}\delta_i^{(x)}\delta_i^{(y)} - x_i\frac{\partial \mu_i^{(x)}}{\partial t}\frac{\partial \delta_i^{(x)}}{\partial x}\delta_i^{(y)} + x_i\frac{\partial w_i}{\partial t}\frac{\partial \delta_i^{(x)}}{\partial x}\delta_i^{(y)} - \frac{\partial \mu_i^{(y)}}{\partial t}\frac{\partial \delta_i^{(y)}}{\partial y}\delta_i^{(x)} + y_i\frac{\partial w_i}{\partial t}\frac{\partial \delta_i^{(y)}}{\partial y}\delta_i^{(x)} = -\frac{\partial}{\partial x}(D_1^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}) - \frac{\partial}{\partial y}(D_2^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}) + \frac{\partial^2}{\partial y^2}(D_{22}^{(2)}w_i\delta_i^{(x)}\delta_i^{(y)})\right]\mathrm{d}x\,\mathrm{d}y\right]. \quad (12)$$

In simplifying Eq. (12) the following properties of the Dirac delta function are used:

$$\int x^r\delta(x-x_i)\,\mathrm{d}x = x_i^r, \quad (13)$$

$$\int x^r\frac{\mathrm{d}\delta(x-x_i)}{\mathrm{d}x}\,\mathrm{d}x = -rx_i^{r-1}. \quad (14)$$

So on using Eqs. (13) and (14) and integrating by parts the right-hand side of Eq. (12) we get the following equation:

$$\begin{aligned}\sum_{i=1}^{M}\Bigg[&x_i^r y_i^s\frac{\partial w_i}{\partial t} + rx_i^{r-1}y_i^s\frac{\partial \mu_i^{(x)}}{\partial t} - rx_i^{r-1}y_i^s x_i\frac{\partial w_i}{\partial t} + sx_i^r y_i^{s-1}\frac{\partial \mu_i^{(y)}}{\partial t}\\ &-sx_i^r y_i^{s-1}y_i\frac{\partial w_i}{\partial t} = -x^r y^s D_1^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}|_{-\infty}^{\infty} + rx_i^{r-1}y_i^s D_1^{(1)}|_{x_i,y_i}w_i\\ &-x^r y^s D_2^{(1)}w_i\delta_i^{(x)}\delta_i^{(y)}|_{-\infty}^{\infty} + sx_i^r y_i^{s-1}D_2^{(1)}|_{x_i,y_i}w_i + x^r y^s\frac{\partial}{\partial y}(D_{22}^{(2)}w_i\delta_i^{(x)}\delta_i^{(y)})|_{-\infty}^{\infty}\\ &-sx^r y^{s-1}D_{22}^{(2)}w_i\delta_i^{(x)}\delta_i^{(y)}|_{-\infty}^{\infty} + s(s-1)x_i^r y_i^{s-2}D_{22}^{(2)}|_{x_i,y_i}\Bigg],\end{aligned} \quad (15)$$

where $|_{x_i,y_i}$ denotes evaluation of the drift and diffusion terms at $x = x_i$ and $y = y_i$. Using the property that the probability density vanishes at positive and negative infinity and the assumption of a smooth probability density function (hence a vanishing derivative of the probability density at positive and negative infinity), the boundary terms in Eq. (15) vanish, leaving after simplification, the following equation:

$$\sum_{i=1}^{M}\left[[1-(r+s)]x_i^r y_i^s \frac{\mathrm{d}w_i}{\mathrm{d}t} + r x_i^{r-1} y_i^s \frac{\mathrm{d}\mu_i^{(1)}}{\mathrm{d}t} + s x_i^r y_i^{s-1}\frac{\mathrm{d}\mu_i^{(2)}}{\mathrm{d}t}\right.$$
$$\left. = r x_i^{r-1} y_i^s D_1^{(1)}|_{x_i,y_i} w_i + s x_i^r y_i^{s-1} D_2^{(1)}|_{x_i,y_i} w_i + s(s-1) x_i^r y_i^{s-2} D_{22}^{(2)}|_{x_i,y_i} w_i\right]. \quad (16)$$

This is now a nonlinear differential equation for each of the weights and weighted abscissas. There are $3M$ such equations, which in matrix form can be written as

$$\mathbf{A}\mathbf{z} = \mathbf{F}(\mathbf{w}, \mathbf{x}, \mathbf{y}), \quad (17)$$

where the matrix $\mathbf{A}$ is a nonlinear function of the abscissas and $\mathbf{z} = \{\mathrm{d}\mathbf{w}/\mathrm{d}t, \mathrm{d}\boldsymbol{\mu}^{(1)}/\mathrm{d}t, \mathrm{d}\boldsymbol{\mu}^{(2)}/\mathrm{d}t\}^{\mathrm{T}}$. Also $\mathbf{w}$, $\mathbf{x}$, $\mathbf{y}$ and $\boldsymbol{\mu}$ are the vectors of weights, abscissas and weighted abscissas, respectively. Eq. (17) is a set of implicit nonlinear ordinary differential equations. In order solve these equations, the DDASPK software package [17–19] is used.

3. Results

Two sample problems are solved to show the effectiveness of the DQMOM solution in solving the Fokker–Planck equation. The first problem is the nonlinear process with stochastic ordinary differential equation given by

$$\mathrm{d}X(t) = (X(t) - X(t)^3)\,\mathrm{d}t + \sigma\,\mathrm{d}W(t), \quad (18)$$

where $\mathrm{d}W(t)$ denotes increments due to a Wiener process and the corresponding Fokker–Planck equation given by

$$\frac{\partial f}{\partial t} = -\frac{\partial}{\partial x}[(x - x^3)f] + \frac{\sigma^2}{2}\frac{\partial^2 f}{\partial x^2}, \quad (19)$$

which we solve numerically using the DQMOM. The deterministic counterpart to this equation ($\mathrm{d}x/\mathrm{d}t = x - x^3$) has two asymptotically stable equilibrium points $x = \pm 1$ separated by an unstable equilibrium point at $x = 0$. An analytical solution to Eq. (19) is not known but the stationary solution is given by

$$P(x) = c\mathrm{e}^{(x^2 - 0.5x^4)/\sigma^2}, \quad (20)$$

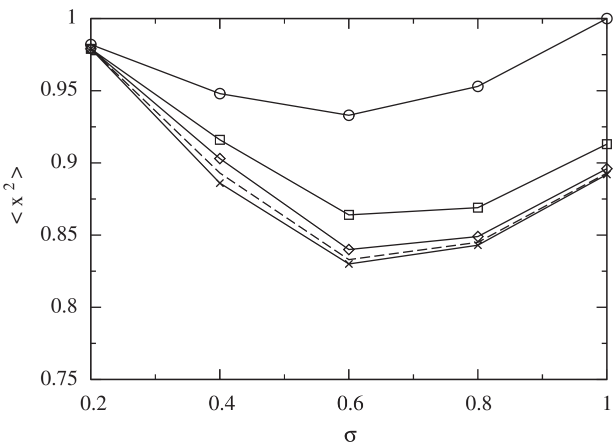

Fig. 1. Second moment of x versus the noise intensity level σ. —○— four quadrature points, —□— six quadrature points, —◇— eight quadrature points, —×— nine quadrature points, - - - analytical.

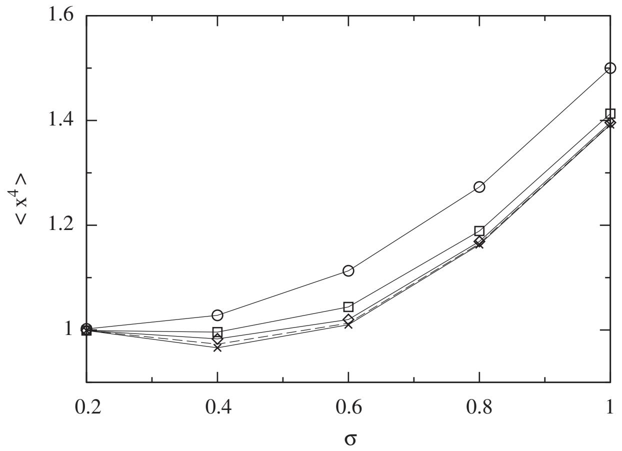

Fig. 2. Fourth moment of x versus the noise intensity level σ. —○— four quadrature points, —□— six quadrature points, —◇— eight quadrature points, —×— nine quadrature points, - - - analytical.

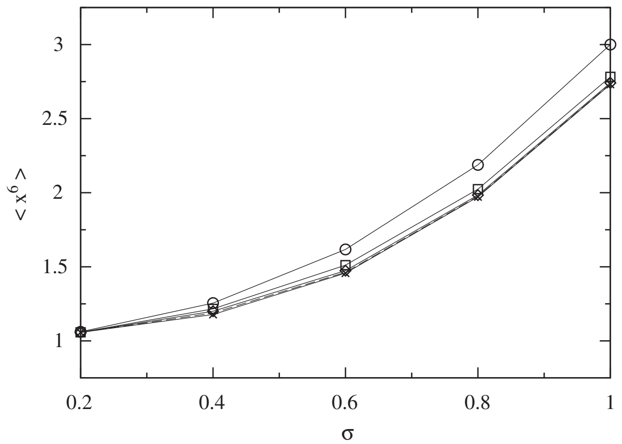

Fig. 3. Sixth moment of x versus the noise intensity level σ. —○— four quadrature points, —□— six quadrature points, —◇— eight quadrature points, —×— nine quadrature points, - - - analytical.

where c is a normalization constant. Figs. 1–3 show the second, fourth and sixth moments as computed by the DQMOM numerical method as a function of the noise level σ. Also shown on these figures are the analytical results computed via Eq. (20). With only eight quadrature nodes the DQMOM and analytical solutions agree quite well for each of the moments. Also note that all odd moments are zero for this problem and the DQMOM method computes these correctly as well.

The second problem which is investigated is the van der Pol oscillator subjected to stationary Gaussian white noise. If the vector process $\mathbf{Z}(t) = \{x(t), y(t)\}^{\mathrm{T}}$ is introduced, where $y(t) = \dot{x}(t)$, the Ito-type stochastic differential equation can be written as

$$\mathrm{d}\mathbf{Z}(t) = \mathbf{f}(\mathbf{Z}(t))\,\mathrm{d}t + \mathbf{Q}\,\mathrm{d}W(t). \tag{21}$$

Here we have

$$\mathbf{f}(\mathbf{Z}(t)) = \left\{ \begin{array}{c} y(t) \\ -\mu[x(t)^2 - 1]y(t) - x(t) \end{array} \right\}, \tag{22}$$

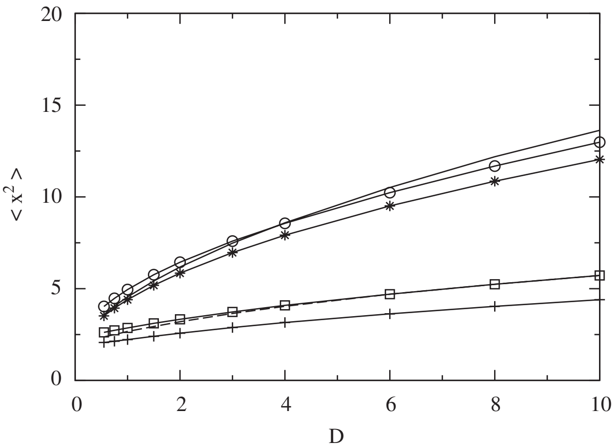

Fig. 4. Second moment of x versus the noise intensity level D. —○— $\mu = 0.1$, eight node direct quadrature method of moments; — $\mu = 0.1$, Monte Carlo; —×— $\mu = 0.1$, statistical nonlinearization [20]; —□— $\mu = 1.0$, eight node direct quadrature method of moments; - - - $\mu = 1.0$, Monte Carlo; —+— $\mu = 1.0$, statistical nonlinearization [20].

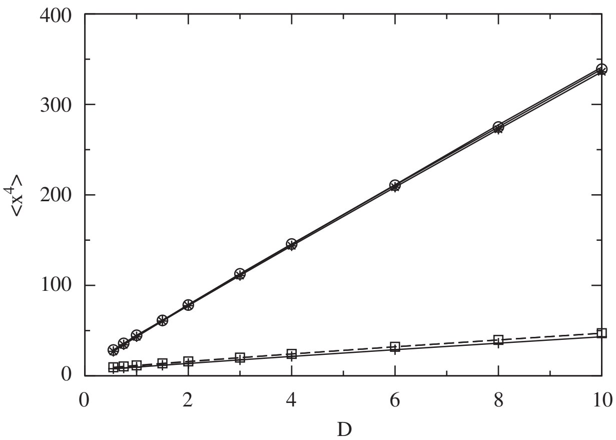

Fig. 5. Fourth moment of x versus the noise intensity level D. —○— $\mu = 0.1$, eight node direct quadrature method of moments; — $\mu = 0.1$, Monte Carlo; —×— $\mu = 0.1$, statistical nonlinearization [20]; —□— $\mu = 1.0$, eight node direct quadrature method of moments; - - - $\mu = 1.0$, Monte Carlo; —+— $\mu = 1.0$, statistical nonlinearization Ref [20].

$$\mathbf{Q} = \begin{Bmatrix} 0 \\ \sqrt{2D} \end{Bmatrix}. \tag{23}$$

The corresponding Fokker–Planck equation for this problem can be written as

$$\frac{\partial f}{\partial t} = \mu(x^2 - 1)f - y\frac{\partial f}{\partial x} + [\mu(x^2 - 1)y + x]\frac{\partial f}{\partial y} + D\frac{\partial^2 f}{\partial y^2}, \tag{24}$$

which is solved numerically using the DQMOM. The second and fourth moments of x as computed by a DQMOM solution of Eq. (24) is shown in Figs. 4 and 5 for $\mu = 0.1$ and 1.0. Also shown in these figures is a numerical solution of the stochastic differential equation, Eq. (21), using a forward Euler–Maruyama time integration scheme. Due to its simplicity, we restricted our attention to the commonly used Euler–Maruyama scheme for integration of stochastic differential equations. It is plausible that high-order integration schemes for stochastic differential equations could lead to more accurate solutions, with greater computational efficiency. The statistics from this solution were computed using a Monte Carlo solution with 5×10^5 particles and a timestep of 0.0005 seconds. These figures also include moments computed using the stationary solutions from the analytic statistical nonlinearization procedure presented in Ref. [20]. In these figures one can see that the second- and fourth-order moments computed using an eight node DQMOM solution compare favorably with the direct solution of the stochastic differential equation. Agreement with the statistical nonlinearization result is better for smaller values of the noise level D and the damping parameter μ which is consistent with the approximations made in the analytic method. Note that in order to compute the DQMOM solution, all moments up to fifth order and $(r, s) = (6, 0)$, (5,1), (4,2) were taken (see Eq. (12)). The DQMOM solution is substantially faster than the direct solution of the stochastic differential equation. On a Intel T2500 2 GHz processor 10 s of simulation time took 4 s of computational time using the DQMOM solution and 1500 s of computational time using the Monte Carlo solution of the stochastic differential equations.

4. Conclusions

A numerical method, the direct quadrature method of moments (DQMOM), is presented for the numerical solution of the Fokker–Planck equation corresponding to stochastic nonlinear dynamical systems. In DQMOM, the probability density function is written as summation of products of Dirac delta functions. The locations of the quadrature abscissas in probability space (arguments of the delta function) become part of the solution and are obtained (along with the quadrature weights) as solutions of their evolution equations. These evolution equations are obtained through the Fokker–Planck equation using constraints on the generalized moments of the stochastic processes. The use of the Dirac delta function results in a much simpler (over traditional weighted-residual methods) treatment of nonlinear drift and diffusion terms.

In this paper the method has been used to compute moments for 1D and 2D processes which possess nonlinear stochastic differential equations. In the 1D problem the stationary moments (second, fourth and sixth) computed using the DQMOM method compare well with analytical solutions. The distribution for this problem is bimodal. The 2D problem was the noisy van der Pol oscillator. Here stationary second- and fourth-order moments computed using the DQMOM solution compared well with those from a direct simulation of the stochastic differential equation and with an analytical solution derived using the statistical nonlinearization procedure.

The authors feel that the method presented possesses the potential to be able to solve high-dimensional Fokker–Planck equations much more efficiently than most current numerical methods. Further work will involve investigating 3D (and higher) stochastic processes in such fields as aeroelasticity and fluid mechanics.

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