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Formulation of a moment method for multidimensional Fokker-Planck equations

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A moment method for general n-dimensional ($n \geq 1$) Fokker-Planck equations in semi-infinite domains with mixed boundary conditions is developed in this paper. Generally, time evolution equations of moments include terms with reduced distribution functions. With mixed boundary conditions in n-dimensional phase spaces, the reduced distribution functions are not explicitly known. This adds an openness to the time evolution equations of moments. We develop an auxiliary set of variables that allow the removal of this type of openness by introducing it into a general moment truncation scheme. The other openness of moment equations caused by the general phase space dependence of drift and diffusion coefficients is removed by using the conventional central moment truncation scheme. The closed set of time evolution equations of moments is numerically solved with the LSODA package of computer programs [A. Hindmarsh, in *Scientific Computing,* edited by R. Stepleman *et al.* (North-Holland, Amsterdam, 1983), pp. 55–64]. The method is applied to three examples. The coupling of moments and reduced moments is first demonstrated by an interstitial clustering process in diatomic materials. Then, the moment equations for a one-dimensional Fokker-Planck equation in a semi-infinite domain are derived as a special case of the present method. The moment equations of the one-dimensional Fokker-Planck equation derived by Ghoniem [Phys. Rev. B **39**, 11 810 (1989)] for atomic clustering are thus recovered in the second example. Finally, the moment method is also tested by applying it to a two-dimensional Ornstein-Uhlenbeck process, which can be solved analytically. Numerical calculations of the first three moments with truncation only at second-order moments are in very good agreement with the analytical results. Truncation at fourth-order moments is found to give similar results for the first three moments.

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I. INTRODUCTION

The Fokker-Planck equation (FPE), which was first developed by Fokker [1] and Planck [2] to describe Brownian motion, has been used in many fields involving stochastic processes. A general review has recently been given by Risken [3]. Analytical solutions can be obtained for very limited conditions, e.g., linear driving force, constant diffusion coefficients, and infinite domains [4–7]. It is generally not possible to obtain analytical solutions of second-order partial differential equations. Many approximate and numerical approaches for the solution of FPEs have already been developed. Some of these methods rely on the specific nature of the equation and many are limited in their range of applications. The reader is referred to procedures based on Lie algebra [8–10], eigenfunction expansion [11–14], perturbation expansion [15–19], path integrals [20–22], Green's function [23–25], Monte Carlo method [26,27], moment method [28–32], and finite difference integration [33–37]. The analytical method is the simplest one, but is usable in a very small class of problems. Numerical integration of a FPE in finite domains could be very accurate with intensive computational efforts. Numerical solutions of multidimensional FPEs in infinite (or semi-infinite) domains are ineffective and may even give false results. The various approximate methods could be very efficient, if their specific assumptions are satisfied.

Although the moment method can be used to solve general FPEs, convergence of the method has not been theoretically proven. However, experience has shown that the method is accurate if one truncates the moment equations at high enough order [38]. The moment method for one-dimensional FPEs has been developed for both infinite and semi-infinite domains [28,29,32], while that for multidimensional FPEs has been developed only for infinite domains [28,32].

Generally, moment equations are not closed. There are two factors that render the moment equations open. First, drift and diffusion coefficients cannot, in general, be expanded in terms of limited order polynomials. This makes the time evolution equations of lower-order moments depend on higher-order moments. A truncation scheme must therefore be employed to eliminate this openness. To obtain moments of up to Nth order, moments of order higher than N need to be omitted or expressed in terms of lower-order moments. This is termed Nth-order truncation or truncation at Nth-order moments. Three truncation schemes have been tested and two of them are found to be good in many cases [30,31]. This openness can therefore be easily removed by using an appropriate truncation scheme.

The other openness comes from mixed boundary conditions (linear combinations of Neumann-type and Dirichlet-type [39] boundary conditions) at finite boundaries in multidimensional phase spaces. For multidimensional Fokker-Planck equations, one mixed boundary condition at a finite boundary gives a governing equation of a reduced distribution function. The reduced distribution function, which is unknown, comes into time evolu-

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tion equations as a boundary condition. Since the reduced distribution is unknown, time evolution equations of moments are rendered open. By introducing an auxiliary set of variables, which we term *reduced moments,* and employing an appropriate truncation scheme, we are able to remove this openness. This paper extends the moment method to more general cases where (1) multidimensional semi-infinite phase spaces are considered and (2) boundary conditions are mixtures of the Neumann and the Dirichlet types. Pure Dirichlet-type boundary conditions are considered as special cases of general mixed boundary conditions.

In Sec. II we develop the moment equations. In Sec. III the moment method is applied to three examples. In the first example, coupling of moments and reduced moments is demonstrated by an interstitial clustering process in diatomic materials. In the second example, the moment equations are applied to the one-dimensional FPE investigated by Ghoniem [29]. The moment equations derived by Ghoniem are recovered as a special case of the present method. Finally, we apply the moment equations to a two-dimensional Ornstein-Uhlenbeck process, where an analytical solution is available. Good agreement between numerical calculations of the moments solved from the moment equations and their analytical counterparts is achieved. The effect of truncation is also investigated. It is found that truncation at fourth-order moments gives similar results of the first three moments as truncation at second-order moments. In Sec. IV we summarize our results and conclusions.

II. MOMENT EQUATIONS

An n-dimensional FPE in a semi-infinite domain is written as

$$\frac{\partial C(\mathcal{N},t)}{\partial t} = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i} F_i(\mathcal{N},t)C(\mathcal{N},t) + \sum_{i,j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(\mathcal{N},t)C(\mathcal{N},t) \qquad (1)$$

with the initial condition

$$C(\mathcal{N},t=0)=C_0(\mathcal{N}) , \qquad (2)$$

the general mixed boundary condition at each finite boundary

$$\frac{\partial u_i(\mathcal{N},t)C(\mathcal{N},t)}{\partial x_i} = v_i(\mathcal{N},t)C(\mathcal{N},t)+w_i(\mathcal{N},t) \quad \text{when } x_i=x_i^* , \qquad (3)$$

and the Dirichlet boundary condition at each infinite boundary

$$C(\mathcal{N},t)=0 \quad \text{as } x_i \to \infty , \qquad (4)$$

where $\mathcal{N}=\{x_1,x_2,\ldots,x_n\}$ is a set of coordinates in the n-dimensional phase space. The asterisk superscript indicates a coordinate at a finite boundary. $F_i(\mathcal{N},t)$ and $D_{ij}(\mathcal{N},t)$ are components of a drift force vector $\mathbf{F}(\mathcal{N},t)$ and a diffusion tensor $\mathsf{D}(\mathcal{N},t)$, respectively. $C(\mathcal{N},t)$ is a distribution function in the n-dimensional phase space and $u_i(\mathcal{N},t)$, $v_i(\mathcal{N},t)$, and $w_i(\mathcal{N},t)$ are arbitrary well-behaved functions.

The boundary conditions defined in Eq. (3) is a mathematical generalization of the following boundary condition:

$$F_i(\mathcal{N},t)C(\mathcal{N},t) - \frac{\partial D_{ii}(\mathcal{N},t)C(\mathcal{N},t)}{\partial x_i} = v_i'(\mathcal{N},t)C(\mathcal{N},t)+w_i(\mathcal{N},t) \quad \text{when } x_i=x_i^* , \qquad (5)$$

which is also a special case of another generalized boundary condition

$$F_i(\mathcal{N},t)C(\mathcal{N},t) - \sum_{j=1}^{n} \frac{\partial D_{ij}(\mathcal{N},t)C(\mathcal{N},t)}{\partial x_j} = v_i'(\mathcal{N},t)C(\mathcal{N},t)+w_i(\mathcal{N},t) \quad \text{when } x_i=x_i^* , \qquad (6)$$

where $v_i'(\mathcal{N},t)$ is another well-behaved function. For this paper, we are satisfied with the boundary condition defined by Eq. (3), which represents defect clustering processes in multicomponent materials.

The general moments $\langle M^{\{m\}} \rangle_{\mathcal{R}}$ are defined by

$$N_{\mathcal{R}} \langle M^{\{m\}} \rangle_{\mathcal{R}} = \int_{\hat{\mathcal{N}}^*}^{\infty} M_{\mathcal{R}}^{\{m\}} C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} , \qquad (7)$$

where $\mathcal{R}=\{x_{r_1}^*,x_{r_2}^*,\ldots,x_{r_d}^*\}$ represents a set of coordinates that will be fixed (reduced). $\hat{\mathcal{N}}$ is a subset defined by $\mathcal{N}=\hat{\mathcal{N}}\oplus\mathcal{R}$. $\{m\}=\{m_1,m_2,\ldots,m_n\}$ is a set of integers that define a specific moment. $N_{\mathcal{R}}$, which is usually termed total number (e.g., total density, total probability), is the integration of the distribution function over a reduced phase space, in which a set of coordinates $\mathcal{R}$ are fixed to be their boundary values. The moment functions $M_{\mathcal{R}}^{\{m\}}$ are defined as

$$M_{\mathcal{R}}^{\{m\}} = \begin{cases} \prod_{i=1}^{n} (x_i - \langle x_i \rangle_{\mathcal{R}})^{m_i} & \text{when } \sum_{k=1}^{n} m_i \neq 1 \\ \prod_{i=1}^{n} x_i^{m_i} & \text{when } \sum_{i=1}^{n} m_i = 1 . \end{cases} \qquad (8)$$

$\sum_{i=1}^{n} m_i=0$ gives the total numbers $N_{\mathcal{R}}$. $\sum_{i=1}^{n} m_i=1$ gives the average values $\langle x_k \rangle_{\mathcal{R}}$. $\sum_{i=1}^{n} m_i=2$ gives the variances $\langle (x_p-\langle x_p \rangle_{\mathcal{R}}(x_q-\langle x_q \rangle_{\mathcal{R}}) \rangle_{\mathcal{R}}$. $\sum_{i=1}^{n} m_i \geq 2$ gives the higher-order moments. When $\mathcal{R}$ is empty, we have the conventional moments. When $\mathcal{R}$ is not an empty set, we have the reduced moments. The order of reduction can be up to $n-1$.

To make the formulation more tractable, we define two operators $\mathbf{I}_{\mathcal{R}}$ and $\mathsf{T}_{\mathcal{R}}$. $\mathbf{I}_{\mathcal{R}}$, which we call the drift vector operator, is defined as

$$\mathbf{I}_{\mathcal{R}} = \sum_{i=1}^{n} I_{\mathcal{R}}^i \mathbf{e}_i , \qquad (9)$$

$$I_{\mathcal{R}}^k f(\hat{\mathcal{N}},\mathcal{R},t) = \int_{\hat{\mathcal{N}}^*}^{\infty} \frac{\partial}{\partial x_k} f(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} \quad \text{if } x_k \in \hat{\mathcal{N}} , \qquad (10)$$

$$I^{r_k}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=\int_{\hat{\mathcal{N}}^*}^{\infty}\frac{\partial}{\partial x^*_{r_k}} f(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} \quad \text{if } x^*_{r_k}\in\mathcal{R}\ , \qquad (11)$$

where $f(\hat{\mathcal{N}},\mathcal{R},t)$ is a well-behaved scalar function. $\mathsf{T}_{\mathcal{R}}$, which we call the diffusion tensor (dyadic) operator, is defined as

$$\mathsf{T}_{\mathcal{R}}=\sum_{i,j=1}^{n} T^{ij}_{\mathcal{R}}\mathbf{e}_i\mathbf{e}_j\ , \qquad (12)$$

$$T^{pq}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=\int_{\hat{\mathcal{N}}^*}^{\infty}\frac{\partial^2}{\partial x_p \partial x_q} f(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} \quad \text{if } x_p,x_q\in\hat{\mathcal{N}}\ , \qquad (13)$$

$$T^{pr_q}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=T^{r_qp}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t) =\int_{\hat{\mathcal{N}}^*}^{\infty}\frac{\partial^2}{\partial x_p \partial x^*_{r_q}} f(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} \quad \text{if } x_p\in\hat{\mathcal{N}},\ x^*_{r_q}\in\mathcal{R}\ , \qquad (14)$$

$$T^{r_pr_q}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=\int_{\hat{\mathcal{N}}^*}^{\infty}\frac{\partial^2}{\partial x^*_{r_p} \partial x^*_{r_q}} f(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} \quad \text{if } x^*_{r_p},x^*_{r_q}\in\mathcal{R}\ . \qquad (15)$$

Operations of the $\mathbf{I}_{\mathcal{R}}$ and $\mathsf{T}_{\mathcal{R}}$ convert a given function into its moments, reduced moments, and some simple integrals, which can be expressed as

$$I^{k}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=-N_{\mathcal{R}_k}\langle f(\hat{\mathcal{N}}_k,\mathcal{R}_k,t)\rangle_{\mathcal{R}_k}\ , \qquad (16)$$

where $\mathcal{R}_k$ is an extended subset defined by $\mathcal{R}_k=\mathcal{R}\oplus\{x^*_k\}$ and $\hat{\mathcal{N}}_k$ is in turn given by

$$\mathcal{N}=\hat{\mathcal{N}}_k\oplus\mathcal{R}_k\ ,$$

$$I^{r_k}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=\begin{cases} +N_{\mathcal{R}}\left\langle \left[u_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)\dfrac{\partial}{\partial x^*_{r_k}}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)}\right]+\dfrac{v_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)}\right]\right\rangle_{\mathcal{R}} \\ \qquad +\displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty}\left[\dfrac{w_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)}\right]d\hat{\mathcal{N}} \quad \text{if } u_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)\neq 0, & (17) \\ -\displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty}\dfrac{\partial}{\partial x^*_{r_k}}\left[\dfrac{w_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)f(\hat{\mathcal{N}},\mathcal{R},t)}{v_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)}\right]d\hat{\mathcal{N}} \quad \text{if } u_{r_k}(\hat{\mathcal{N}},\mathcal{R},t)=0\ , & (18) \end{cases}$$

$$T^{pq}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=N_{\mathcal{R}_{pq}}\left\langle f(\hat{\mathcal{N}}_{pq},\mathcal{R}_{pq},t)\right\rangle_{\mathcal{R}_{pq}} \quad \text{if } p\neq q\ ,\ x_p,x_q\in\hat{\mathcal{N}}\ , \qquad (19)$$

where $\mathcal{R}_{pq}$ is another extended subset defined by $\mathcal{R}_{pq}=\mathcal{R}\oplus\{x^*_p,x^*_q\}$ and $\hat{\mathcal{N}}_{pq}$ is in turn given by $\mathcal{N}=\hat{\mathcal{N}}_{pq}\oplus\mathcal{R}_{pq}$,

$$T^{pp}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=\begin{cases} -N_{\mathcal{R}_p}\left\langle u_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)\dfrac{\partial}{\partial x^*_p}\left[\dfrac{f(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}{u_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}\right]+\dfrac{v_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)f(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}{u_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}\right\rangle_{\mathcal{R}_p} \\ \qquad -\displaystyle\int_{\hat{\mathcal{N}}^*_p}^{\infty}\left[\dfrac{w_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)f(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}{u_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}\right]d\hat{\mathcal{N}}_p \quad \text{if } u_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)\neq 0, & (20) \\ +\displaystyle\int_{\hat{\mathcal{N}}^*_p}^{\infty}\dfrac{\partial}{\partial x^*_p}\left[\dfrac{w_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)f(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}{v_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}\right]d\hat{\mathcal{N}}_p \quad \text{if } u_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)=0\ , & (21) \end{cases}$$

$$T^{pr_q}_{\mathcal{R}} f(\hat{\mathcal{N}},\mathcal{R},t)=\begin{cases} -N_{\mathcal{R}_p}\left\langle u_{r_q}(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)\dfrac{\partial}{\partial x^*_{r_q}}\left[\dfrac{f(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}{u_{r_q}(\mathcal{N}_p,\mathcal{R}_p,t)}\right]+\dfrac{v_{r_q}(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)f(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}{u_{r_q}(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}\right\rangle_{\mathcal{R}_p} \\ \qquad -\displaystyle\int_{\hat{\mathcal{N}}^*_p}^{\infty}\left[\dfrac{2_{r_q}(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)f(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}{u_{r_q}(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}\right]d\hat{\mathcal{N}}_p \quad \text{if } u_{r_q}(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)\neq 0, & (22) \\ +\displaystyle\int_{\hat{\mathcal{N}}^*_p}^{\infty}\dfrac{\partial}{\partial x^*_{r_q}}\left[\dfrac{w_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)f(\mathcal{N}_p,\mathcal{R}_p,t)}{v_p(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)}\right]d\hat{\mathcal{N}}_p \quad \text{if } u_{r_q}(\hat{\mathcal{N}}_p,\mathcal{R}_p,t)=0\ , & (23) \end{cases}$$

$$
T_{\mathcal{R}}^{r_p r_p} f(\hat{\mathcal{N}},\mathcal{R},t) = \begin{cases}
+N_{\mathcal{R}}\left\langle u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)\dfrac{\partial^2}{\partial x_{r_p}^{*2}}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\right] + \dfrac{v_{r_p}^2(\hat{\mathcal{N}},\mathcal{R},t) f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}^2(\hat{\mathcal{N}},\mathcal{R},t)}\right\rangle_{\mathcal{R}} \\
\quad + N_{\mathcal{R}}\left\langle 2v_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)\dfrac{\partial}{\partial x_{r_p}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\right] + f(\hat{\mathcal{N}},\mathcal{R},t)\dfrac{\partial}{\partial x_{r_p}^*}\left[\dfrac{v_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\right]\right\rangle_{\mathcal{R}} \\
\quad + \displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t) v_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) w_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}^2(\hat{\mathcal{N}},\mathcal{R},t)} + \dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)\partial w_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)\partial x_{r_p}^*}\right] d\hat{\mathcal{N}} \\
\quad + \displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty} 2w_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)\dfrac{\partial}{\partial x_{r_p}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\right]\hat{\mathcal{N}} \quad \text{if } u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) \neq 0, & (24) \\
-\displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty}\dfrac{\partial^2}{\partial x_{r_p}^{*2}}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t) w_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}{v_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\right] d\hat{\mathcal{N}} \quad \text{if } u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) = 0\ , & (25)
\end{cases}
$$

$$
T_{\mathcal{R}}^{r_p r_q} f(\hat{\mathcal{N}},\mathcal{R},t) = \begin{cases}
+N_{\mathcal{R}}\left\langle u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)\dfrac{\partial}{\partial x_{r_p}^*}\left[\dfrac{u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\dfrac{\partial}{\partial x_{r_p}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}\right]\right]\right\rangle_{\mathcal{R}} \\
\quad + N_{\mathcal{R}}\left\langle u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)\dfrac{\partial}{\partial x_{r_p}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t) v_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}\right]\right\rangle_{\mathcal{R}} \\
\quad + N_{\mathcal{R}}\left\langle \dfrac{v_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\dfrac{\partial}{\partial x_{r_q}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}\right]\right\rangle_{\mathcal{R}} \\
\quad + N_{\mathcal{R}}\left\langle \dfrac{f(\hat{\mathcal{N}},\mathcal{R},t) v_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) v_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}\right\rangle_{\mathcal{R}} \\
\quad + \displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t) v_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) w_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)} + \dfrac{\partial}{\partial x_{r_p}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t) w_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}\right]\right] d\hat{\mathcal{N}} \\
\quad + \displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty}\dfrac{u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t) w_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t)}\dfrac{\partial}{\partial x_{r_q}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t)}{u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}\right] d\hat{\mathcal{N}} \\
\quad\quad \text{if } r_p \neq r_q\ ,\ u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t) \neq 0 & (26) \\
-\displaystyle\int_{\hat{\mathcal{N}}^*}^{\infty}\dfrac{\partial^2}{\partial x_{r_p}^*\partial x_{r_q}^*}\left[\dfrac{f(\hat{\mathcal{N}},\mathcal{R},t) w_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}{v_{r_q}(\hat{\mathcal{N}},\mathcal{R},t)}\right] d\hat{\mathcal{N}} \quad \text{if } r_p \neq r_q\ ,\ u_{r_p}(\hat{\mathcal{N}},\mathcal{R},t) u_{r_q}(\hat{\mathcal{N}},\mathcal{R},t) = 0\ . & (27)
\end{cases}
$$

The derivation of these equations is straightforward and is therefore omitted here. Using the drift and diffusion operators, we can express time evolution equations of the moments in the following compact form:

$$
\begin{aligned}
\frac{d[N_{\mathcal{R}}\langle M^{\{m\}}\rangle_{\mathcal{R}}]}{dt} &= +N_{\mathcal{R}}\left\langle\left[\mathbf{F}(\hat{\mathcal{N}},\mathcal{R},t) - \left[\frac{d\langle\mathcal{N}\rangle_{\mathcal{R}}}{dt}\right]\Gamma\left[\sum_{k=1}^{n} m_i - 2\right]\right]\cdot\mathbf{Y}_{\mathcal{R}} M_{\mathcal{R}}^{\{m\}}\right\rangle_{\mathcal{R}} \\
&\quad + N_{\mathcal{R}}\left\langle \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)\cdot\cdot\mathsf{Z}_{\mathcal{R}} M_{\mathcal{R}}^{\{m\}}\right\rangle_{\mathcal{R}} + \mathsf{T}_{\mathcal{R}}\cdot\cdot[\mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t) M_{\mathcal{R}}^{\{m\}}] \\
&\quad - \mathbf{I}_{\mathcal{R}}\cdot\{[\mathbf{F}(\hat{\mathcal{N}},\mathcal{R},t) + \mathbf{Y}_{\mathcal{R}}\cdot\mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t) + \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)\cdot\mathbf{Y}_{\mathcal{R}}] M_{\mathcal{R}}^{\{m\}}\}\ ,
\end{aligned} \tag{28}
$$

where

$$\mathbf{Y}_{\mathcal{R}}=\sum_{i=1}^{n}\frac{m_i}{(x_i-\langle x_i\rangle_{\mathcal{R}})}\mathbf{e}_i \ , \tag{29}$$

$$\mathbf{Z}_{\mathcal{R}}=\sum_{i,j=1}^{n}\frac{m_i(m_j-\delta_{ij})}{(x_i-\langle x_i\rangle_{\mathcal{R}})(x_j-\langle x_j\rangle_{\mathcal{R}})}\mathbf{e}_i\mathbf{e}_j \ , \tag{30}$$

$$\frac{d\langle\mathcal{N}\rangle_{\mathcal{R}}}{dt}=\sum_{\substack{i=1\\ x_i\in\hat{\mathcal{N}}}}\frac{d\langle x_i\rangle_{\mathcal{R}}}{dt}\mathbf{e}_i \ , \tag{31}$$

$$\Gamma(\chi)=\begin{cases}1 & \text{if } \chi\ge 0\\ 0 & \text{if } \chi<0 \ .\end{cases} \tag{32}$$

Details of the derivation for Eq. (28) are given in the Appendix. The reduced distribution functions, which are included in time evolution equations of moments, and can be expanded in terms of their moments and reduced moments. By introducing the reduced moments and employing an appropriate truncation scheme, we have closed the openness caused by mixed boundary conditions at finite boundaries. Generally, the drift vector and the diffusion tensor are expansions of infinite-order polynomials of their phase space coordinates. This makes time evolution equations of lower-order moments depend on higher-order moments. Therefore, the time evolution equations of lower-order moments are generally not closed. This openness can be removed by truncating the time evolution equations at an appropriate order. There are several truncation schemes proposed [30,31]: simple moment truncation, central moment truncation, and cumulant truncation. By applying the truncation procedures to some analytically solvable processes, it has been found that the central moment truncation and cumulant truncation schemes are more accurate as compared to the simple moment truncation scheme. For general FPEs, the central moment truncation scheme is easier than the cumulant truncation scheme and will therefore be adopted in this work. The moment equations, which are a set of ordinary differential equations, can be easily solved with the LSODA package of computer programs [40,41].

III. APPLICATIONS OF THE MOMENT METHOD

In Sec. III A, coupling of the moments and the reduced moments is demonstrated by an interstitial atoms clustering process in diatomic materials. Moment equations for one-dimensional FPEs in a semi-infinite domain developed by Ghoniem [29] are recovered as a special case in Sec. III B. Numerical accuracy of the method is demonstrated in Sec. III C by applying it to a two-dimensional Ornstein-Uhlenbeck process, for which an analytical solution is available.

A. Interstitial atom clustering processes in diatomic materials

When defects are produced in a solid, they tend to form clusters. According to the two-group approach [38], defects (vacancies, interstitials, and their clusters) are described by two sets of equations: small defects are described by master equations and large defects are described by a FPE. This approach has been extended to defect clustering processes in diatomic materials and applied to silicon carbide [42]. The two sets of equations can be expressed as

$$\frac{dC_1}{dt}=f_1\{C_1,C_2C(x_1,x_2,t),\alpha\} \ , \tag{33}$$

$$\frac{dC_2}{dt}=f_2\{C_1,C_2,C(x_1,x_2,t),\alpha\} \ , \tag{34}$$

$$\frac{dC_{11}}{dt}=f_{11}\{C_1,C_2,C(x_1,x_2,t),\alpha\} \ , \tag{35}$$

$$\frac{\partial C(x_1,x_2,t)}{\partial t}=-\sum_{i=1}^{2}\frac{\partial}{\partial x_i}F_i(x_1,x_2,t)C(x_1,x_2,t)+\sum_{i,j=1}^{2}\frac{\partial^2}{\partial x_1\partial x_j}D_{ij}(x_1,x_2,t)C(x_1,x_2,t) \ , \tag{36}$$

$$F_i(x_1,x_2,t)C(x_1,x_2,t)-\frac{\partial}{\partial x_i}D_{ii}(x_1,x_2,t)C(x_1,x_2,t)=A_i(x_1,x_2,t)C(x_1,x_2,t) \quad \text{at } x_i=1 \ , \tag{37}$$

$$C(\infty,x_2,t)=C(x_1,\infty,t)=0 \ , \tag{38}$$

$$C(x_1,x_2,0)=\text{known function of } x_1 \text{ and } x_2 \ , \tag{39}$$

$$C(1,1,t)=C_{11} \ , \tag{40}$$

where f_1, f_2, and f_{11} are known functionals. α represents all material properties and damage conditions. $A_i(x_1,x_2,t)$ is a known function. C_1, C_2, and C_{11} are concentrations of type-A interstitials, type-B interstitials, and stoichiometric di-interstitials, respectively, while $C(x_1,x_2,t)$ represents concentration of defect clusters. The di-interstitials are described by both the master equations and the FPE.

The FPE can be converted to a set of moment equations as described in Sec. II. Simultaneously solving the moment equations and master equations, we can get a distribution of defect clusters. Details of this physical problem are discussed in Ref. [42]. Coupling of the moments and the reduced moments is highlighted through the equation for zeroth-order (nonreduced) moment

$$\begin{aligned}\frac{dN}{dt}&=T^{11}D_{11}(x_1,x_2,t)+T^{22}D_{22}(x_1,x_2,t)\\&\quad+T^{12}D_{12}(x_1,x_2,t)+T^{21}D_{21}(x_1,x_2,t)\\&\quad-I^1F_1(x_1,x_2,t)-I^2F_2(x_1,x_2,t) \ ,\end{aligned} \tag{41}$$

where

$$I^1F_1(x_1,x_2,t)=-N_{\{x_1^*\}}\langle F_1(x_1^*,x_2,t)\rangle_{\{x_1^*\}} \ , \tag{42}$$

$$I^2F_2(x_1,x_2,t)=-N_{\{x_2^*\}}\langle F_1(x_1,x_2^*,t)\rangle_{\{x_2^*\}} \ , \tag{43}$$

$$T^{11}D_{11}(x_1,x_2,t)=-N_{\{x_1^*\}}\langle F_1(x_1^*,x_2,t)-A_1(x_1^*,x_2,t)\rangle_{\{x_1^*\}} \ , \tag{44}$$

$$T^{22}D_{22}(x_1,x_2,t) = -N_{\{x_2^*\}}\langle F_2(x_1,x_2^*,t)-A_2(x_1,x_2^*,t)\rangle_{\{x_2^*\}} , \quad (45)$$

$$T^{12}D_{12}(x_1,x_2,t)=D_{12}(x_1^*,x_2^*,t)C_{11} , \quad (46)$$

$$T^{21}D_{21}(x_1,x_2,t)=D_{21}(x_1^*,x_2^*,t)C_{11} . \quad (47)$$

It is clear that the reduced average terms have to be expanded in terms of the reduced moments. The zeroth-order moment N is therefore shown to be coupled with the reduced moments. Similarly, higher-order moments are also coupled with the reduced moments. Equations for the moments and the reduced moments and the master equations have to be solved simultaneously to obtain defect distribution functions.

B. One-dimensional FPE in semi-infinite domains

Considering the one-dimensional FPE in a semi-infinite domain studied by Ghoniem [29], we can write the boundary conditions as

$$u(x,t)=D(x,t) , \quad (48)$$

$$w(x,t)=-\frac{dN}{dt} , \quad (49)$$

$$v(x,t)=F(x,t) . \quad (50)$$

Substituting these boundary conditions into the right-hand side of Eq. (28), we have

$$\frac{dN}{dt}=F(x^*,t)C(x^*,t)-\frac{dD(x^*,t)C(x^*,t)}{dx^*} , \quad (51)$$

$$\frac{d\langle x\rangle}{dt}=\langle F(x,t)\rangle-(\langle x\rangle-x^*)\frac{d\ln N}{dt}+\frac{D(x^*,t)C(x^*,t)}{N} , \quad (52)$$

$$\frac{d\langle M^{\{m\}}\rangle}{dt}=m\langle(x-\langle x\rangle)^{m-1}F(x,t)\rangle+m(m-1)\langle(x-\langle x\rangle)^{m-2}D(x,t)\rangle + \frac{m(x^*-\langle x\rangle)^{m-1}D(x^*,t)C(x^*,t)}{N}+\frac{d\ln N[(x^*-\langle x\rangle)^m-\langle M^{\{m\}}\rangle]}{dt}-m\langle M^{\{m-1\}}\rangle\frac{d\langle x\rangle}{dt} . \quad (53)$$

These equations are precisely the same as Eqs. (23), (25), and (27) in Ref. [29], except for the use of different symbols. The moment equations are solved simultaneously with several master equations describing small defects [29]. It is worth mentioning that there are two matching boundary conditions at the finite boundary x^* because both $C(x,t)$ and its first-order spatial derivative are continuous in order to be physically meaningful. Since they are matching boundary conditions, the problem is mathematically well posed.

C. Ornstein-Uhlenbeck process

A simple Ornstein-Uhlenbeck process in a two-dimensional infinite phase space can be described by the following set of equations:

$$\frac{\partial C(x_1,x_2,t)}{\partial t}=-\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left[\sum_{k=1}^{2}a_{ik}x_k\right]C(x_1,x_2,t) + \sum_{i,j=1}^{2}\frac{\partial^2}{\partial x_i\partial x_j}D_{ij}C(x_1,x_2,t) , \quad (54)$$

$$C(x_1,x_2,t=0)=\delta(x_1-1)\delta(x_2-1) , \quad (55)$$

$$C(x_1,x_2,t)=0 \quad \text{as } x_i\to\infty , \quad (56)$$

where $\delta(x)$ is the Dirac delta function. In this example a_{ik} and D_{ij} are constants. We take $a_{ik}=\delta_{ik}$ and $D_{ij}=10^{-2}\delta_{ij}$, with δ_{ij} being the Kroneker delta function.

This problem can be solved analytically and the distribution function can be expressed as [3]

$$C(x_1,x_2,t)=\frac{1}{0.02\pi(e^{2t}-1)} \times\exp\left[\frac{(x_1-e^t)^2+(x_2-e^t)^2}{0.02(e^{2t}-1)}\right] . \quad (57)$$

It is easy to prove that this is also the solution of the same FPE in a semi-infinite domain, which is defined as $x_1\in(x_1^*,\infty)$ and $x_2\in(x_2^*,\infty)$, if we choose the following boundary functions at the finite boundaries:

$$u_i(x_1,x_2,t)=1.0 , \quad (58)$$

$$v_i(x_1,x_2,t)=-\frac{x_i-e^t}{10^{-2}(e^{2t}-1)} , \quad (59)$$

$$w_i(x_1,x_2,t)=0.0 , \quad (60)$$

where i can be 1 or 2 depending on which boundary is considered.

Moments of this distribution function in the semi-infinite domain can be directly calculated. With the chosen boundary functions, we can also solve for the moments using the method developed in Sec. II. Moments calculated from the analytical solution at $t=5.0$ with $x_1^*=100$ and $x_2^*=100$ are used as initial conditions for the moment equations. The time dependence of the moments is studied by both the moment method and the analytical distribution function. Truncating the moment equations at the second-order moments, we have solved for the first three moments. Because the problem is symmetrical with the two coordinates, we do not need to

TABLE I. Effects of truncation on the accuracy of $\langle M^{\{m\}}\rangle - \langle M^{\{m\}}\rangle_{t=5.0}$.

Moment m_1, m_2	$\langle M^{\{m\}}\rangle - \langle M^{\{m\}}\rangle_{t=5.0}$ Analytical	Second order	Fourth order	$E_0^{\{m\}}$ (%) Second order	Fourth order
0, 0	1.1054×10^{-3}	1.1049×10^{-3}	1.1049×10^{-3}	0.05	0.05
1, 0	9.6250×10^{1}	9.6250×10^{1}	9.6250×10^{1}	0.00	0.00
2, 0	3.7988×10^{2}	3.7988×10^{2}	3.7988×10^{2}	0.00	0.00
3, 0	-6.1622×10^{1}		3.4314×10^{3}		5668.47
4, 0	9.3412×10^{5}		9.7683×10^{5}		4.57
2, 2	3.1058×10^{5}		3.1058×10^{5}		0.00

consider moments of all coordinates. The time dependence of the total number obtained from the moment method and that of its analytical counterpart are compared in Fig. 1. Similar comparisons for average values and variances are shown in Figs. 2 and 3, respectively. The approximate moments obtained using the moment method agree very well with their exact counterparts. To study the effects of truncation, moments and their relative errors are calculated with various orders of truncation as

$$E_0^{\{m\}} = \left|\frac{(\langle M^{\{m\}}\rangle - \langle M^{\{m\}}\rangle_{t=5.0})_{\text{approximate}} - (\langle M^{\{m\}}\rangle - \langle M^{\{m\}}\rangle_{t=5.0})_{\text{analytical}}}{(\langle M^{\{m\}}\rangle - \langle M^{\{m\}}\rangle_{t=5.0})_{\text{analytical}}}\right|_0 , \tag{61}$$

where $E_0^{\{m\}}$ represents relative error of moment increase $\langle M^{\{m\}}\rangle - \langle M^{\{m\}}\rangle_{t=5.0}$, with zeroth-order truncation. The subscript $t=5.0$ indicates initial values of moments. Nonzero moments and their relative errors, at $t=5.5$, for truncation of second and fourth orders are calculated and listed in Table I. The moments that have an analytically zero value are not included in Table I since the magnitude of all their approximate values is less than 10^{-4}. The results of lower-order moments are stable with respect to truncation at two different orders. The large relative error for a third moment is due to the fact that its analytical value is very small. In this case, contributions of higher-order moments dominate and truncation causes a large relative error.

It is worth mentioning that we chose the boundary function $v_i(x_1,x_2,t) = -(x_i - e^t)/10^{-2}(e^{2t}-1)$ to obtain an analytical solution. This function, however, is singular when $t=0.0$. Therefore, $t=5.0$ rather than $t=0.0$ is taken as a starting time to avoid numerical difficulties.

IV. CONCLUSIONS AND REMARKS

In this work, the moment method is developed for n-dimensional FPEs in semi-infinite domains with mixed boundary conditions. The idea introduced here can be directly applied to deriving moment equations of n-dimensional FPEs in finite domains with mixed boundary

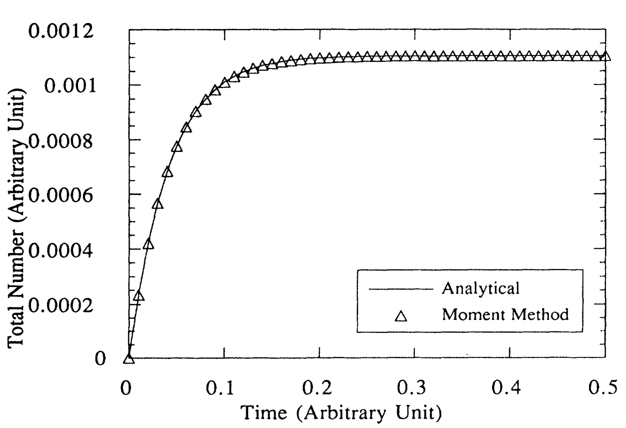

FIG. 1. Comparison of the total number solved from the moment equations with its analytical counterpart. The moment increase $N - N_{t=t_0}$ is plotted against the time increase $t - t_0$. The initial values are $t_0 = 5.0$ and $N_{t=t_0} = 0.998\,894\,631\,9$.

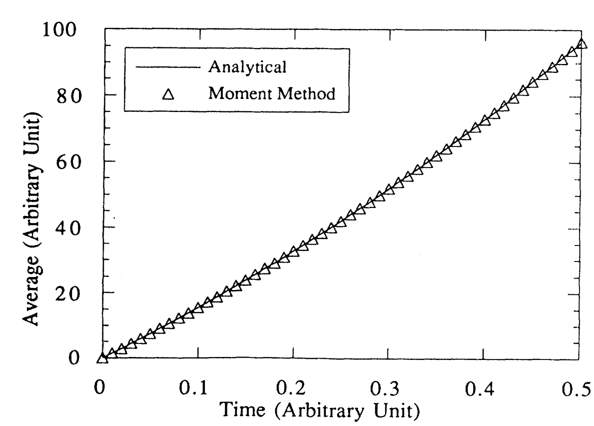

FIG. 2. Comparison of the average value of x_1 solved from the moment equations with its analytical counterpart. The moment increase $\langle x_1\rangle - \langle x_1\rangle_{t=t_0}$ is plotted against the time increase $t - t_0$. The initial values are $t_0 = 5.0$ and $\langle x_1\rangle_{t=0} = 148.442\,123\,4$.

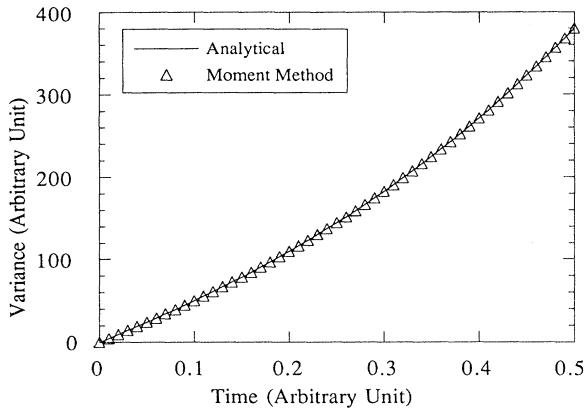

FIG. 3. Comparison of the variance of x_1 solved from the moment equations with its analytical counterpart. The moment increase $\langle (x_1-\langle x_1\rangle)^2\rangle - \langle (x_1-\langle x_1\rangle)^2\rangle_{t=t_0}$ is plotted against the time increase $t-t_0$. The initial values are $t_0=5.0$ and $\langle (x_1-\langle x_1\rangle)^2\rangle_{t=t_0}=218.851\,608\,3$.

conditions, whenever necessary. Several salient conclusions can be drawn based on this work.

(i) The moment equations for one-dimensional FPEs derived by Ghoniem are recovered as a special case of the general moment method developed in this paper.

(ii) With truncation at second-order moments, the moment equations accurately predict time evolution of the first three moments of a simple two-dimensional Ornstein-Ohlenbeck process. The relative errors are less than 0.05%.

(iii) With truncation at fourth-order moments, the moment equations give the same prediction accuracy of the first three moments as truncation at second-order moments. On the other hand, prediction of a third-order moment is in large relative error with its analytical counter part. This can be accounted for by the fact that this moment is very small compared to higher-order moments. Therefore higher-order moments dominate and truncation causes larger errors.

(iv) From results obtained with truncation of different orders, we suggest that convergence of moments should be tested for each problem. This can be done by solving for first several moments at various orders of truncation.

There are several ways of constructing a distribution function based on known moments. Choosing a reconstruction scheme may introduce some uncertainties. Since in many cases the first three moments (or higher-order moments) give enough information of a random process, we will not discuss construction of distribution functions in this paper. The method developed here can be applied to many fields involving FPEs, particularly defect clustering theory for multicomponent materials [42].

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APPENDIX: DERIVATION OF THE MOMENT EQUATIONS

$$\frac{dN_{\mathcal{R}}\langle M^{\{m\}}\rangle_{\mathcal{R}}}{dt} = \int_{\hat{\mathcal{N}}^*}^{\infty} \prod_{i=1}^{n} (x_i-\langle x_i\rangle_{\mathcal{R}})^{m_i} \left[-\sum_{j=1}^{n} \frac{\partial F_j(\hat{\mathcal{N}},\mathcal{R},t)}{\partial x_j} + \sum_{j,l=1}^{n} \frac{\partial^2 D_{il}(\hat{\mathcal{N}},\mathcal{R},t)}{\partial x_j \partial x_l} \right] C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}}$$
$$- \int_{\hat{\mathcal{N}}^*}^{\infty} \sum_{j=1}^{n} \frac{m_j}{(x_j-\langle x_j\rangle_{\mathcal{R}})} \frac{d\langle x_j\rangle_{\mathcal{R}}}{dt} \prod_{k=1}^{n} (x_i-\langle x_i\rangle_{\mathcal{R}})^{m_i} C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} \ . \qquad \text{(A1)}$$

The second term does not exist for zeroth- and first-order moments. For higher-order moments, it can be written as

$$- \int_{\hat{\mathcal{N}}^*}^{\infty} \sum_{j=1}^{n} \frac{m_j}{(x_j-\langle x_j\rangle_{\mathcal{R}})} \frac{d\langle x_j\rangle_{\mathcal{R}}}{dt} \prod_{i=1}^{n} (x_i-\langle x_i\rangle_{\mathcal{R}})^{m_i} C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}} = -N_{\mathcal{R}} \left\langle \frac{d\langle\mathcal{N}\rangle_{\mathcal{R}}}{dt} \cdot \mathbf{Y}_{\mathcal{R}} M_{\mathcal{R}}^{\{m\}} \right\rangle_{\mathcal{R}} \ . \qquad \text{(A2)}$$

The drift term can be expressed in terms of moments as

$$- \int_{\hat{\mathcal{N}}^*}^{\infty} \prod_{i=1}^{n} (x_i-\langle x_i\rangle \mathcal{R})^{m_i} \sum_{j=1}^{n} \frac{\partial}{\partial x_j} F_j(\hat{\mathcal{N}},\mathcal{R},t) C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}}$$
$$= - \int_{\hat{\mathcal{N}}^*}^{\infty} \sum_{j=1}^{n} \frac{\partial}{\partial x_j} F_j(\hat{\mathcal{N}},\mathcal{R},t) \prod_{i=1}^{n} (x_i-\langle x_i\rangle_{\mathcal{R}})^{m_i} C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}}$$
$$+ \int_{\hat{\mathcal{N}}^*}^{\infty} \sum_{j=1}^{n} \frac{m_j}{(x_j-\langle x_j\rangle_{\mathcal{R}})} F_j(\hat{\mathcal{N}},\mathcal{R},t) \prod_{i=1}^{n} (x_i-\langle x_i\rangle_{\mathcal{R}})^{m_i} C(\hat{\mathcal{N}},\mathcal{R},t)d\hat{\mathcal{N}}$$
$$= -\mathbf{I}_{\mathcal{R}} \cdot \mathbf{F}(\hat{\mathcal{N}},\mathcal{R},t) M_{\mathcal{R}}^{\{m\}} + N_{\mathcal{R}} \langle \mathbf{F}(\hat{\mathcal{N}},\mathcal{R},t) \cdot \mathbf{Y}_{\mathcal{R}} M_{\mathcal{R}}^{\{m\}} \rangle_{\mathcal{R}} \ . \qquad \text{(A3)}$$

For the diffusion term, if $j \neq 1$, we have

$$\frac{\partial^2}{\partial x_l \partial x_j}[(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$=+(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}\frac{\partial^2}{\partial x_l \partial x_j}[D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$+m_l m_j(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l-1}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-1}D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)$$

$$+m_j(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-1}\frac{\partial}{\partial x_1}[D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$+m_l(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l-1}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}\frac{\partial}{\partial x_j}[D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$=+(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}\frac{\partial^2}{\partial x_l \partial x_j}[D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$-m_l m_j(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l-1}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-1}D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)$$

$$+m_j\frac{\partial}{\partial x_l}[(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-1}D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$+m_l\frac{\partial}{\partial x_j}[(x_l-\langle x_l\rangle_{\mathcal{R}})^{m_l-1}(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]\ . \tag{A4}$$

If $j=1$, we have

$$\frac{\partial^2}{\partial x_j^2}[x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}D_{jj}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$=+(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}\frac{\partial^2}{\partial x_j^2}[D_{jj}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$+m_j(m_j-1)(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-2}D_{jj}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)+2m_j(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-1}\frac{\partial}{\partial x_j}[D_{jj}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$=+(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j}\frac{\partial^2}{\partial x_j^2}[D_{jj}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]$$

$$-m_j(m_j-1)(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-2}D_{jj}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)+2m_j\frac{\partial}{\partial x_j}[(x_j-\langle x_j\rangle_{\mathcal{R}})^{m_j-1}D_{jj}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)]\ . \tag{A5}$$

Therefore

$$\int_{\hat{\mathcal{N}}*}^{\infty}\prod_{i=1}^{n}(x_i-\langle x_i\rangle_{\mathcal{R}})^{m_i}\sum_{\substack{j=1\\ l\neq j}}\frac{\partial^2 D_{jl}(\hat{\mathcal{N}},\mathcal{R},t)C(\hat{\mathcal{N}},\mathcal{R},t)}{\partial x_j \partial x_l}d\hat{\mathcal{N}}$$

$$=+N_{\mathcal{R}}\langle \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},\mathsf{T})\cdot\cdot \mathsf{Z}_{\mathcal{R}}M_{\mathcal{R}}^{\{m\}}\rangle_{\mathcal{R}}+\mathsf{T}_{\mathcal{R}}\cdot\cdot \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)-\mathbf{I}_{\mathcal{R}}\cdot\cdot[\mathbf{Y}_{\mathcal{R}}\cdot \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)+\mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)\cdot \mathbf{Y}_{\mathcal{R}}]M_{\mathcal{R}}^{\{m\}}\ . \tag{A6}$$

If $(x_i-\langle x_i\rangle_{\{r_d\}})$ is replaced by x_i or 1, the above formulation is unchanged, except that the last term in Eq. (A1) disappears. Therefore, we have

$$\frac{d\{N_{\mathcal{R}}\langle M^{\{m\}}\rangle_{\mathcal{R}}\}}{dt}=+\left\langle\left[\mathbf{F}(\hat{\mathcal{N}},\mathcal{R},t)-\frac{d\langle\mathcal{N}\rangle_{\mathcal{R}}}{dt}\Gamma\left[\sum_{i=1}^{n}m_i-2\right]\right]\cdot \mathbf{Y}_{\mathcal{R}}M_{\mathcal{R}}^{\{m\}}\right\rangle_{\mathcal{R}}$$

$$+N_{\mathcal{R}}\langle \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)\cdot\cdot \mathsf{Z}_{\mathcal{R}}M_{\mathcal{R}}^{\{m\}}\rangle_{\mathcal{R}}+\mathsf{T}_{\mathcal{R}}\cdot\cdot \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)M_{\mathcal{R}}^{\{m\}}$$

$$-\mathbf{I}_{\mathcal{R}}\cdot[\mathbf{F}(\hat{\mathcal{N}},\mathcal{R},t)+\mathbf{Y}_{\mathcal{R}}\cdot \mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)+\mathsf{D}(\hat{\mathcal{N}},\mathcal{R},t)\cdot \mathbf{Y}_{\mathcal{R}}]M_{\mathcal{R}}^{\{m\}}\ . \tag{A7}$$

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