Title: The Mori-Zwanzig Approach to Uncertainty Quantification

Name: Daniele Venturi[1], Heyrim Cho[2], George Em Karniadakis[3]

Affil./Addr. 1: Department of Applied Mathematics and Statistics

University of California Santa Cruz

Santa Cruz, CA 95064

E-mail: venturi@ucsc.edu

Affil./Addr. 2: Department of Mathematics

University of Maryland

College Park, MD 20742

Affil./Addr. 3: Division of Applied Mathematics

Brown University

Providence, RI 02912

The Mori-Zwanzig Approach to Uncertainty Quantification

Summary. Determining the statistical properties of nonlinear random systems is a problem of major interest in many areas of physics and engineering. Even with recent theoretical and computational advancements, no broadly applicable technique has yet been developed for dealing with the challenging problems of high dimensionality, low regularity and random frequencies often exhibited by the system. The Mori-Zwanzig and the effective propagator approaches discussed in this chapter have the potential of overcoming some of these limitations, in particular the curse of dimensionality and the lack of regularity. The key idea stems from techniques of irreversible statistical mechanics, and it relies on developing exact evolution equations and corresponding numerical methods for quantities of interest, e.g., functionals of the solution to stochastic ordinary and partial differential equations. Such quantities of interest could be low-dimensional objects in infinite dimensional phase spaces, e.g., the lift of an airfoil in a turbulent flow, the local displacement of a structure subject to random loads (e.g., ocean

waves loading on an offshore platform) or the macroscopic properties of materials with random microstructure (e.g., modeled atomistically in terms of particles). We develop the goal-oriented framework in two different, although related, mathematical settings: the first one is based on the Mori-Zwanzig projection operator method and it yields exact reduced-order equations for the quantity of interest. The second approach relies on effective propagators, i.e., integrals of exponential operators with respect to suitable distributions. Both methods can be applied to nonlinear systems of stochastic ordinary and partial differential equations subject to random forcing terms, random boundary conditions or random initial conditions.

Introduction

Experiments on high-dimensional random systems provide observations of macroscopic phase variables such as the mass density in Newtonian fluids, the stress-strain relation in heterogeneous random materials (e.g., carbon-fiber) or the velocity distribution in granular flows. These quantities can be related to a thorough microscopic description of the system by taking averages of real valued (measurable) functions defined on a very high-dimensional phase space . To understand the dynamics of such phase space functions one often wishes to obtain closed equations of motion by eliminating the rest of the degrees of freedom. One of the most typical examples for such contraction of state variables is the derivation of the Boltzmann equation from the Newton's law or from the Liouville equation [143; 119; 16]. Another example of a different type is the Brownian motion of a particle in a liquid, where the master equation governing the position and momentum of the particle is derived from first principles (Hamilton equations of motion of the full system), by eliminating the degrees of freedom of the liquid [68; 17]. In stochastic systems far from equilibrium, one often has to deal with the problem of eliminating macroscopic phase variables, i.e., phase variables with the same order of magnitude and dynamical properties as the ones of interest. For example, to define the turbulent viscosity in the inertial range of fully developed turbulence, one

has to eliminate short wavelength components of the fluid velocity which are far from equilibrium. This problem arises more often than one would expect, and it is more challenging than the problem of contracting microscopic phase variables. For example, it arises when deriving the master equation for the series expansion of the solution to a nonlinear stochastic partial differential equation (SPDE), given any discretized form.

In this chapter we illustrate how to perform the contraction of state variables in non-equilibrium stochastic dynamical systems by using the Mori-Zwanzig projection operator method and the effective propagator approach. In particular, we will show how to develop computable evolution equations for quantities of interest in high-dimensional stochastic systems and how to determine their statistical properties. This problem received considerable attention in recent years. Well-known approaches to compute such properties are generalized polynomial chaos (gPC) [51; 155; 156], multi-element generalized polynomial chaos (ME-gPC) [147; 139], multi-element and sparse adaptive probabilistic collocation (ME-PCM) [44; 45; 85; 33], high-dimensional model representations [113; 77], stochastic biorthogonal expansions [132; 138; 133] and generalized spectral decompositions [101; 102]. These techniques can provide considerable speed-up in computational time when compared to classical approaches such as Monte Carlo (MC) or quasi-Monte Carlo methods. However, there are still several important computational limitations that have not yet been overcome. They are related to:

1. *High-Dimensionality:* Many problems of interest to physics and engineering can be modeled mathematically in terms of systems of nonlinear ODEs or nonlinear PDEs subject to random initial conditions, random parameters, random forcing terms or random boundary conditions. The large number of phase variables involved in these problems plus the high-dimensionality of the random input vectors poses major computational challenges in representing the stochastic solution , e.g., in terms of polynomial chaos or probabilistic collocation. In fact, the number of terms in poly-

nomial chaos series expansions or the number of collocation points in probabilistic collocation methods, grows exponentially fast with the number of dimensions (in tensor product discretizations).

2. *Low Stochastic Regularity:* The computational cost of resolving solutions with *low stochastic regularity* is also an issue. Parametric discontinuities can create Gibbs-type phenomena which can completely destroy the convergence numerical methods - just like in spectral methods [58; 103]. Parametric discontinuities are *unavoidable* in nonlinear systems and they are often associated with interesting physics, e.g., around bifurcation points [139; 140]. By using adaptive methods, e.g., ME-gPC or ME-PCM, one can effectively resolve such discontinuities and restore convergence. This is where "h-refinement" in parameter space is particularly important [145; 44].
3. *Multiple Scales:* stochastic systems can involve multiple scales in space, time and phase space (see Fig. 1) which could be difficult to resolve by conventional numerical methods.
4. *Long-Term Integration:* The flow map defined by systems of differential equations can yield large deformations, stretching and folding of the phase space. As a consequence, methods that represent the parametric dependence of the solution on random input variables, e.g., in terms of polynomials chaos of fixed order or in terms of a fixed number of collocation points, will lose accuracy as time increases. This phenomenon can be mitigated, although not completely overcome, by using multi-element methods [146; 44], time-evolving bases [118], or a composition of short-term flow maps [81].

The Mori-Zwanzig and the effective propagator approaches have the potential of overcoming some of these limitations, in particular the curse of dimensionality and the lack of regularity.

Overcoming High Dimensions

The Mori-Zwanzig and the effective propagator approaches allow us for a *systematic elimination* of the "irrelevant" degrees of freedom of the system, and they yield formally exact equations for quantities of interest, e.g., functionals of the solution to high-dimensional systems of stochastic ordinary differential equations (SODEs) and stochastic partial differential equations (SPDEs). This allows us to *avoid integrating the full (high-dimensional) stochastic dynamical system* and solve directly for the quantities of interest. In principle, this can break the curse of dimensionality in numerical simulations of SODEs and SPDEs at the price of solving complex integro-differential PDEs - the Mori-Zwanzig equations. The computability of such PDEs relies on approximations. Over the years many methods have been proposed for this scope. For example, small correlation expansions [122; 31; 47], cumulant resummation methods [137; 46; 17; 13; 79], functional derivative techniques [141; 54; 53; 52], path integral methods [154; 131; 87; 109], decoupling approximations [55] and local linearization methods [36]. However, these techniques are not, in general, effective in eliminating degrees of freedom with the *same order of magnitude and dynamical properties* as the quantities of interest. Several attempts have been made to overcome these limitations and establish a computable framework for Mori-Zwanzig equations that goes beyond closures based on perturbation analysis. We will discuss some of these methods later in this chapter.

Overcoming Low Regularity

The PDF of low-dimensional quantities of interest depending on many phase variables is usually a *regular function*. This is due to a *homogenization effect* induced by multi-dimensional integration. In other words, the PDF of low-dimensional quantities of interest is often not just low-dimensional but also *smooth*, i.e., amenable to compu-

tation. As an example, consider the joint PDF of the Fourier coefficients of a turbulent flow. It is known that such joint PDF lies on an attractor with a possibly fractal structure [43; 50; 42]. However, the linear combination of the Fourier modes, i.e. the Fourier representation of the velocity field at a specific space-time location, turns out to be approximately Gaussian. This behavior is exhibited by other chaotic dynamical systems such as the Lorentz-96 system [80] evolving from a random initial state. In this case, it can be shown that the joint PDF of the phase variables approaches asymptotically in time a fractal attractor whose dimension depends on the amplitude of the forcing term (see, e.g., [70]). However, the marginal distributions of such complex joint PDF are approximately Gaussian (see Fig. 4).

Formulation

Let us consider the nonlinear dynamical system

$$\begin{cases} \dfrac{dx(t;\omega)}{dt} = f(x(t;\omega), \xi(\omega), t) \\ x(0;\omega) = x_0(\omega) \end{cases}, \tag{1}$$

where $x(t;\omega) \in \mathbb{R}^n$ is a multi-dimensional stochastic process, $f : \mathbb{R}^{n+m+1} \to \mathbb{R}^n$ is a deterministic nonlinear map assumed to be Lipschitz continuous in x, $\xi(\omega) \in \mathbb{R}^m$ is a random vector modeling input uncertainty, and $x_0(\omega) \in \mathbb{R}^n$ is a random initial state. The system (1) can be very large as it can arise, e.g., from a discretization of a nonlinear SPDE. We assume that the solution to (1) exists and is it is unique for each realization of $\xi(\omega)$ and $x_0(\omega)$. This allows us to consider $x(t;\omega)$ as a deterministic function of $\xi(\omega)$ and $x_0(\omega)$, i.e., we can define the parametrized *flow map* $\widehat{x}(t;\xi(\omega), x_0(\omega))$. The joint PDF of $x(t;\omega)$ and $\xi(\omega)$ can be represented as

$$p(a,b,t) = \langle \delta(a - \widehat{x}(t;\xi;x_0))\delta(b-\xi) \rangle, \quad a \in \mathbb{R}^n, \quad b \in \mathbb{R}^m, \tag{2}$$

where $\langle\cdot\rangle$ denotes an integral with respect to the joint probability distribution of $\xi(\omega)$ and $x_0(\omega)$, while δ are multi-dimensional Dirac delta functions [72; 69]. Also, the vectors a and b represent the phase space coordinates corresponding to $x_i(t;\omega)$ and $\xi(\omega)$ respectively. By differentiating (2) with respect to time and using well-known identities involving the Dirac delta function it is straightforward to obtain the following exact hyperbolic conservation law

$$\frac{\partial p(a,b,t)}{\partial t} = L(a,b,t)p(a,b,t), \qquad L(a,b,t) = -\sum_{i=1}^{n}\left(\frac{\partial f_i(a,b,t)}{\partial a_i} + f_i\frac{\partial}{\partial a_i}\right). \tag{3}$$

In the sequel we will often set $p(t) \equiv p(a,b,t)$ and $L(t) \equiv L(a,b,t)$ for notational convenience. Equation (3) is equivalent to the Liouville equation of classical statistical mechanics (for non-Hamiltonian systems), with the remarkable difference that the phase variables we consider here can be rather general coordinates - not simply positions and momenta of particles. For instance, they could be the Galerkin or the collocation coefficients arising from a spatial discretization of a SPDE, e.g., if we represent the solution as

$$u(X,t;\omega) = \sum_{j=1}^{n} x_j(t;\omega)\phi_j(X), \tag{4}$$

where $\phi_j(X)$ are spatial basis functions. Early formulations in this direction were proposed by Edwards [34], Herring [57] and Montgomery [91] in the context of fluid turbulence .

Some Properties of the Solution to the Joint PDF Equation

Nonlinear systems in the form (1) can lead to all sorts of dynamics, including bifurcations, fractal attractors, multiple stable steady states and transition scenarios. Consequently, the solution to the joint PDF equation (3) can be very complex as well, since it relates directly to the geometry of the phase space. For example, it is known that the time-asymptotic joint PDF associated with the Lorentz three-mode problem lies on a fractal attractor with Hausdorff dimension of about 2.06 (see [144]). Chaotic

states and existence of strange attractors has been well documented for many other systems, such as the Lorenz-84 see [14] and the Lorenz-96 [70] models. Even in the much simpler case of the Duffing equation

$$\frac{dx_1}{dt} = x_2, \qquad \frac{dx_2}{dt} = -x_1 - 5x_1^3 - \frac{x_2}{50} + 8\cos\left(\frac{t}{2}\right) \tag{5}$$

we can have attractors with fractal structure and chaotic phase similarities [11]. This is clearly illustrated in Fig. 1 where we plot the Poincaré sections of the two-dimensional phase space at different times. Such sections are obtained by sampling 10^6 initial states from a zero-mean jointly Gaussian distribution, and then evolving them by using (5). Since the joint PDF of the phase variables is, in general, a high-dimensional compactly supported distribution with a possibly fractal structure, its numerical approximation is a very challenging task, especially in long time integration.

However, the statistical description of the system (1) in terms of the joint PDF equation (3) is often far beyond practical needs. For instance, we may be interested only in the PDF of only one component, e.g. $x_1(t;\omega)$, or in the PDF of a phase space function $u = g(x)$ such as (4). These PDFs can be obtained either by integrating out several phase variables from the solution to Eq. (3), by constructing NARMAX models (see [7] §5.7) or by applying the projection operator or the effective propagator approaches discussed in this chapter. This may yield a *low-dimensional* PDF equation whose solution is *more regular* than the one obtained by solving directly Eq. (3), and therefore more amenable to computation. The regularization of the reduced-order PDF is due to multi-dimensional integration (marginalization) of the joint PDF.

Dimension Reduction: BBGKY Hierarchies

A family of reduced-order probability density functions can be obtained by integrating the solution to Eq. (3) with respect to the phase space coordinates which are not of

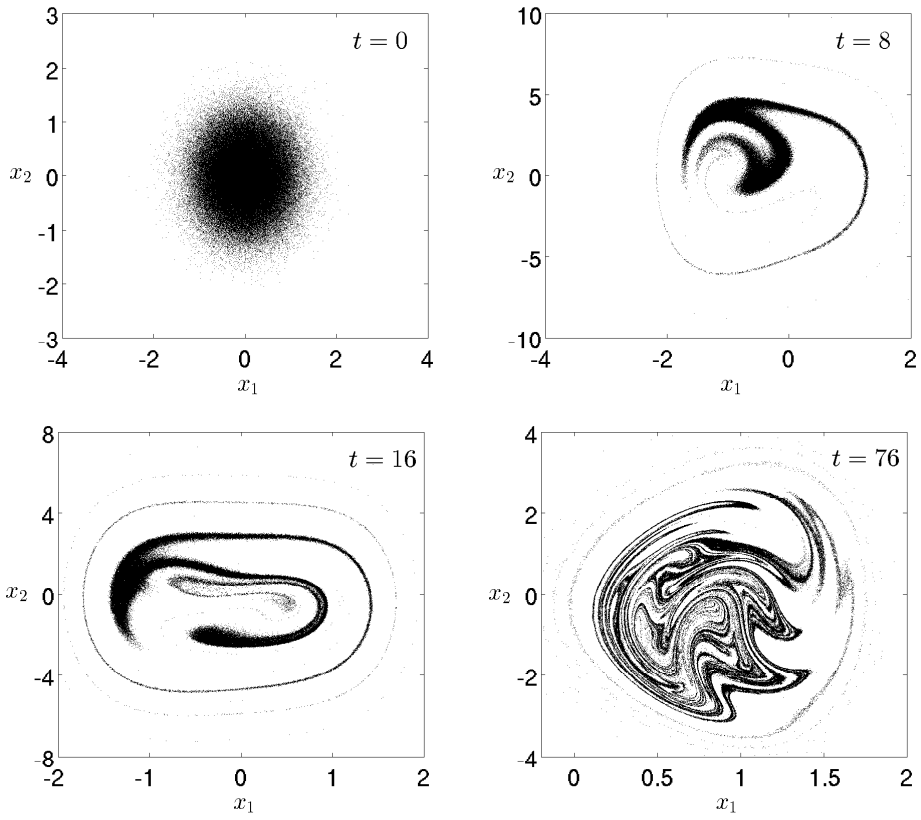

Fig. 1. Duffing equation. Poincaré sections of the phase space at different times obtained by evolving a zero-mean jointly Gaussian distribution with covariance $C_{11} = C_{22} = 1/4$, $C_{12} = 0$. Note that simple statistical properties such as the mean and variance are not sufficient to describe the stochastic dynamics of the system (5). (Adapted from [137]).

interest. This yields, for example,

$$p_i(a_i, t) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} p(a, b, t) da_1 \cdots da_{i-1} da_{i+1} \cdots da_n db, \qquad i = 1, .., n. \tag{6}$$

These reduced-order densities differ from those used in classical BBGKY theory [16], mainly in that they are not, in general, symmetric under interchanges of different phase space coordinates. For instance, $p_i(a_i, t)$ is not the same function of a_i that $p_j(a_j, t)$ is of a_j, if i and j are different. In the classical BBGKY framework the phase coordinates of the systems are positions and momenta of identical particles. Therefore, the reduced-order multi-point densities are invariant under interchanges of phase space coordinates of the same type, e.g., positions or momenta. Most of the added complexity to the classical BBGKY theory stems from this lack of symmetry. A related approach,

due to Lundgren [82] and Monin [90], yields a hierarchy of PDF equations involving suitable limits of reduced density functions (see also [135; 136; 60; 49; 153]). The effective computability of both BBGKY-type and Lundgren-Monin hierarchies arising from Eq. (3) relies in appropriate closure schemes, e.g., a truncation based on a suitable decoupling approximation of the PDF. In particular, the mean-field approximation

$$p(t,a,b) = p_\xi(b)\prod_{i=1}^{n} p_i(a_i,t), \tag{7}$$

where $p_\xi(b)$ is the joint PDF of the random vector ξ, yields the system of conservation laws ($i = 1, ..., n$)

$$\frac{\partial p_i(a_i,t)}{\partial t} = -\frac{\partial}{\partial a_i}\left[p_i(a_i,t)\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} f_i(a,b,t)p_\xi(b)\prod_{\substack{j=1\\ j\neq i}}^{n} p_j(a_j,t)da_j db\right]. \tag{8}$$

These equations are coupled through the integrals appearing within the square bracket. As an example, consider the Lorentz-96 system [70]

$$\frac{dx_i}{dt} = (x_{i+1} - x_{i-2})\,x_{i-1} - x_i + c, \qquad i = 1, ..., 40. \tag{9}$$

The first-order truncation of the BBGKY hierarchy is ($i = 1, ..., 40$)

$$\frac{\partial p_i(a_i,t)}{\partial t} = -\frac{\partial}{\partial a_i}\left[\left(\langle x_{i+1}\rangle - \langle x_{i-2}\rangle\right)\langle x_{i-1}\rangle\, p_i(a_i,t) - (a_i - c)p_i(a_i,t)\right], \tag{10}$$

where $\langle\cdot\rangle$ denotes averaging with respect to the joint PDF of the system, assumed in the form (7). Higher-order truncations, i.e., truncations involving multi-point PDFs can be obtained in a similar way (see [22; 91]). Clearly, higher truncation orders yield better accuracy, but at higher computational cost (see Fig. 2).

The Mori-Zwanzig Projection Operator Framework

The basic idea of the Mori-Zwanzig formalism is to reduce the dimensionality of the dynamical system (1) by splitting the phase variables into two categories: the *relevant*

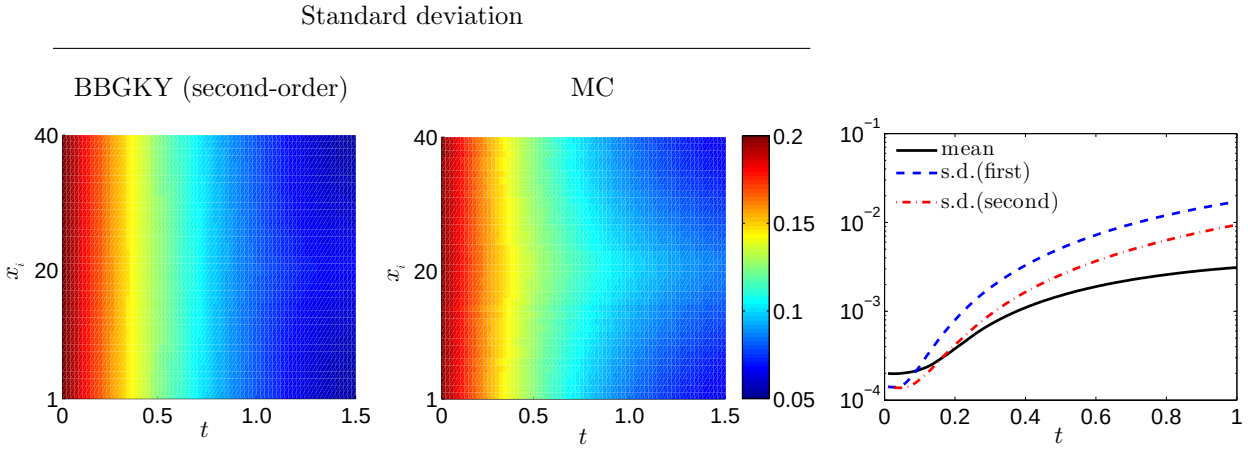

Fig. 2. Lorenz-96 system: Standard deviation of the phase variables versus time (left) and absolute errors of first- and second-order truncations of the BBGKY hierarchy relative to MC. (Adapted from [22])

(or resolved) variables and the *irrelevant* (or unresolved) ones. These two sets can be easily classified by means of an orthogonal projection operator P that maps the state vector onto the set of resolved variables. By applying such orthogonal projection to Eq. (3) it is straightforward to obtain the following exact equation

$$\frac{\partial Pp(t)}{\partial t} = PL(t)Pp(t) + PL(t)G(t,0)Qp(0) + PL(t)\int_0^t G(t,s)QL(s)Pp(s)ds, \quad (11)$$

first derived by Nakajima [97], Zwanzig [159; 160] and Mori [92]. Here we have set $p(t) \equiv p(a,b,t)$ and $L(t) \equiv L(a,b,t)$ for notational convenience, and denoted by $Q = I - P$ the projection onto the unresolved variables. The operator $G(t,s)$ (forward propagator of the orthogonal dynamics) is formally defined as

$$G(t,s) = \overleftarrow{T} \exp\left[\int_s^t QL(\tau)d\tau\right], \quad (12)$$

where $\overleftarrow{T}$ is the chronological time-ordering operator (latest times to the left). For a detailed derivation see, e.g., [137; 160; 13; 17; 67]. From Eq. (11) we see that the exact dynamics of the PDF of the relevant phase variables (projected PDF $Pp(t)$) depends on three terms: the *Markovian term* $PL(t)Pp(t)$ - computable based on the current state $Pp(t)$; the *initial condition (or noise) term* $PL(t)G(t,0)Qp(0)$ and the *memory*

term (time convolution), both depending on the propagator $G(t,0)$ of the orthogonal dynamics. The critical part of the MZ formulation is to find reliable and accurate approximations of the memory and the initial condition terms.

The nature of the projection operator P will be discussed extensively in subsequent sections. For now, it is sufficient to note that such projection basically extracts from the full joint PDF equation (3) only the part that describes (in an exact way) the dynamics of the relevant phase variables. A simple analysis of Eq. (11) immediately shows its irreversibility. Roughly speaking, the projected distribution function $Pp(t)$, initially in a certain subspace, leaks out of this subspace so that information is lost, hence the memory (time convolution) and the initial condition terms.

Coarse-Grained Dynamics in the Phase Space

The Mori-Zwanzig projection operator method just described can be also used to reduce the dimensionality of either deterministic or stochastic *systems of equations in the phase space*, yielding generalized Langevin equations [119; 62] for quantities of interest. One remarkable example of such equations is the one describing the *coarse-grained dynamics* of a particle system. Within this framework the phase variables $x_i(t)$ in (1) can represent either the position or the momentum of the particle "i". Coarse-graining is achieved by defining a new set of state variables

$$u(t;\omega) = g\left(x(t;\omega), t\right) \qquad \text{(quantities of interest)} \tag{13}$$

where $g : \mathbb{R}^{n+1} \to \mathbb{R}^q$ is a a phase space function and q is usually much smaller than n. These variables can represent the position or the momentum of entire *clusters of particles*, e.g, the big green particles shown in Fig. 3. The irrelevant phase variables in this case are the components of the full state vector x. The generalized Langevin equation satisfied by (13) can be obtained by using standard methods [119; 95; 30; 62].

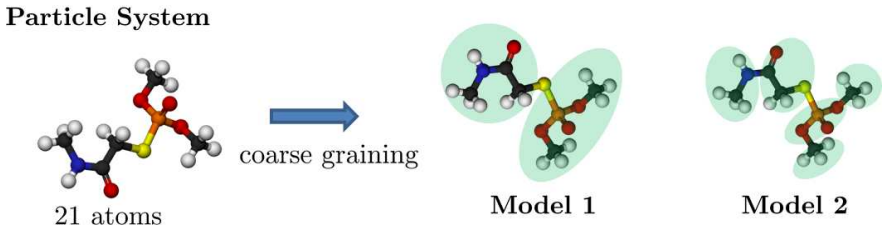

Fig. 3. Coarse graining particle systems using the projection operator method. The microscopic degrees of freedom associated with each atom are condensed into a smaller number of degrees of freedom (those associated with the big green particles). Coarse-graining is not unique, and therefore fundamental questions regarding model inadequacy, selection and validation have to be carefully addressed.

For example, if the system is autonomous, i.e., if the right hand side of Eq. (1) reduces to $f(x)$, then we have the formally exact coarse-grained system (see [93; 62; 158])

$$\frac{du_i(t)}{dt} = e^{tM}PMu_i(0) + \int_0^t e^{(t-s)M}PMR_i(s)ds + R_i(t), \qquad i = 1, ..., q \tag{14}$$

where P is an orthogonal projection operator and

$$M = \sum_{j=1}^{n} f_j(x_0)\frac{\partial}{\partial x_0}, \qquad R_i(t) = e^{t(I-P)M}(I-P)Mu_i(t). \tag{15}$$

The state-space reduced order equations (14) are particularly useful if $u_i(t)$ is a complete set of slowly varying variables relative to the dynamics of the unresolved variables, i.e., the dynamics of $x(t;\omega)$. In this case, the fluctuating forces $R_i(t)$ are rapidly varying in time due to their modified propagator $\exp[t(I-P)M]$ and the memory kernel rapidly decays to zero. Effective approximations are possible in these cases [66; 62; 78; 158]. Based on the phase space formulation, it is also possible to obtain the Mori-Zwanzig equation for the one-point or the multi-point PDF of the quantities of interest (13). To this end, it is sufficient to differentiate the distribution function

$$p_u(a,t) = \langle \delta(a - u(t;\omega)) \rangle \,, \tag{16}$$

with respect to time and substitute (14) within the average (see, e.g., [93; 119] for the derivation). If (1) represents the semi-discrete form of a SPDEs and we are interested in the phase space function (4), then the Mori-Zwanzig formulation yields the *exact*

PDF equation for the series expansion of the solution to the SPDE. This overcomes the well-known *closure problem* arising in PDF equations corresponding to SPDEs with diffusion or higher-order terms [106; 142; 111]. On the other hand, if $u_i(t) = x_i(t)$ $(i = 1, ..., q)$ are the first q components of a Galerkin dynamical system then the Mori-Zwanzig projection operator method allows us to construct a closure approximation in which the *unresolved dynamics* (modes from $q+1$ to n) is injected in a *formally exact way* into the *resolved dynamics*. This use of projection operators has been investigated, e.g., by Chorin [27; 24], Stinis [120] and Chertok [20]. Early studies in this direction - not involving Mori-Zwanzig - employed *inertial manifolds* [41] and *nonlinear Galerkin projections* [84].

Projection Operators

The coarse graining of the microscopic equations of motion can be performed by introducing a projection operator and applying it to the master equation (3) (coarse graining in the PDF space - Eq. (11)) or to the dynamical system (1) (coarse-graining in the phase space - Eq. (14)). Well-known choices are the Zwanzig projection [160], the Mori projection, projections defined in terms of Boltzmann-Gibbs measures [119; 62; 129] or projections defined by conditional expectations [27; 30; 25; 120]. If the relevant and the irrelevant phase variables (hereafter denoted by a and b, respectively) are statistically independent, i.e., if $p(0) = p_a(0)p_b(0)$, then a convenient projection is

$$Pp(t) = p_b(0) \int p(t)db \quad \Rightarrow \quad p_a(t) = \int Pp(t)db. \tag{17}$$

This projection takes the joint PDF $p(t)$ and basically sends it to a separated state. In this case we have that $p(0)$ is in the range of P, i.e., $Pp(0) = p(0)$, and therefore the initial condition term in the MZ-PDF equation drops out since $Qp(0) = (I-P)p(0) = 0$.

Time-Convolutionless Form of the Mori-Zwanzig Equation

The Mori-Zwanzig PDF (MZ-PDF) equation (11) can be transformed into a Markovian (time-convolutionless) form. To this end, we simply consider the formal solution to orthogonal dynamics equation

$$Qp(t) = G(t,0)Qp(0) + \int_0^t G(t,s)QL(s)Pp(s)ds, \tag{18}$$

and replace $p(s)$ with the solution to Eq. (3), propagated backward from time t to time $s < t$, i.e.

$$p(s) = Z(t,s)p(t), \qquad \text{where} \qquad Z(t,s) = \overrightarrow{T} \exp\left[-\int_s^t L(\tau)d\tau\right]. \tag{19}$$

In the latter definition $\overrightarrow{T}$ is the anti-chronological ordering operator (latest times to the right). Substituting (19) into (18) yields

$$Qp(t) = [I - \Sigma(t)]^{-1} G(t,0)Qp(0) + [I - \Sigma(t)]^{-1} \Sigma(t)Pp(t), \tag{20}$$

where

$$\Sigma(t) = \int_0^t G(t,s)QL(s)PZ(t,s)ds. \tag{21}$$

Equation (20) states that the "irrelevant" part of the PDF $Qp(t)$ can, in principle, be determined from the knowledge of the "relevant" part $Pp(t)$ at time t, and from the initial condition $Qp(0)$. Thus, the dependence on the history of the relevant part which occurs in the classical Mori-Zwanzig equation has been removed by the introduction of the backward propagator (19). By using the orthogonal dynamics equation (20), we obtain the Markovian (time-convolutionless) MZ-PDF equation

$$\frac{\partial Pp(t)}{\partial t} = K(t)Pp(t) + H(t)Qp(0), \tag{22}$$

where

$$K(t) = PL(t)\,[I - \Sigma(t)]^{-1}, \qquad H(t) = PL(t)\,[I - \Sigma(t)]^{-1}\,G(t,0). \tag{23}$$

Many other equivalent forms of the Mori-Zwanzig equation can be constructed (see the Appendix in [137]), exactly for the same reason as why it is possible to represent an effective propagator of reduced-order dynamics in terms of generalized operator cumulants [56; 98; 75; 74]. So far, everything that has been said is exact, and it led us to the equation of motion (22), which is linear and local in time. Unfortunately, such equation is still of little practical use, because the exact determination of the operators K and H is as complicated as the solution of Eq. (3). However, the time-convolutionless form (22) is a convenient starting point to construct *systematic approximation schemes*, e.g., by expanding K and H in terms of cumulant operators relative to suitable coupling constants [108; 17; 13; 116; 75; 65; 67; 98].

Multi-Level Coarse-Graining in Probability and Phase Spaces

In [137] we recently proposed a multi-level coarse graining technique in which the evolution equation for the orthogonal PDF dynamics $Qp(t)$

$$\frac{\partial Qp(t)}{\partial t} = QL(t)[Pp(t) + Qp(t)], \tag{24}$$

is decomposed further by introducing a new pair of orthogonal projections P_1 and Q_1 such that $P_1 + Q_1 = I$. This yields the coupled system

$$\frac{\partial P_1 Qp(t)}{\partial t} = P_1 QL(t)\left[Pp(t) + P_1 Qp(t) + Q_1 Qp(t)\right], \tag{25}$$

$$\frac{\partial Q_1 Qp(t)}{\partial t} = Q_1 QL(t)\left[Pp(t) + P_1 Qp(t) + Q_1 Qp(t)\right]. \tag{26}$$

Proceeding similarly, we can split the equation for $Q_1 Qp(t)$ by using a new pair of orthogonal projections P_2 and Q_2 satisfying $P_2 + Q_2 = I$. This yields two additional evolution equations for $P_2 Q_1 Qp(t)$ and $Q_2 Q_1 Qp(t)$, respectively. Obviously, one can repeat this process indefinitely to obtain a hierarchy of equations which *generalizes* both the Mori-Zwanzig as well as the BBGKY frameworks. The advantage of this formulation with respect to the classical approach relies on the fact that the joint PDF

$p(t)$ is not simply split into the "relevant" and the "irrelevant" parts by using P and Q. Indeed, the dynamics of the irrelevant part $Qp(t)$ is decomposed further in terms of a new set of projections.

This allows us to coarse-grain relevant features of the orthogonal dynamics further in terms of lower-dimensional quantities. In other words, the *multi-level projection operator method* allows us to *seemingly interface dynamical systems at different scales in a mathematically rigorous way.* This is particularly useful when coarse graining (in state space) high-dimensional systems in the form (1). To this end, we simply have to define a set of quantities of interest $u^{(1)} = g^{(1)}(x,t)$, $u^{(2)} = g^{(2)}(x,t)$, etc. (see (13)), e.g., representing clusters of particles of different sizes, and corresponding projection operators P_1, P_2, etc. This yields a coupled set of equations resembling (14) in which relevant features of the microscopic dynamics are interacting at different scales defined by different projection operators.

The Closure Problem

Most schemes that attempt to compute the solution of MZ equations or BBGKY-type hierarchies rely on the identification of some small quantity that serves as the basis for a perturbation expansion, e.g., the density for Boltzmann equations [16], the coupling constant or correlation time for Fokker-Planck-type equations [122; 31; 47; 94] or the Kraichnan absolute equilibrium distribution for turbulent inviscid flows [91; 73]. One of the most stubborn impediments for the development of a general theory of reduced-order PDF equations has been the lack of such readily identifiable small parameters. Most of the work that has been done so far refers to the situation in which such small parameters exist, e.g., when the operator L in Eq. (3) can be decomposed as

$$L = L_0 + \sigma L_1. \tag{27}$$

Here L_0 depends only on the relevant variables of the system, σ is a positive real number (coupling constant in time-dependent quantum perturbation theory) and the norm $\sigma \|L_1\|$ is somehow *small* (see, e.g., [13; 94; 17]). By using the interaction representation of quantum mechanics [150; 9], then it is quite straightforward to obtain from (22) and (27) an effective approximation (see [137]). One way to do so is to expand the operators (23) in a cumulant series, e.g., in terms of Kubo-Van Kampen operator cumulants [56; 75; 65; 98], involving increasing powers of σ (coupling parameter). Any finite-order truncation of such series then represents an *approximation* to the exact MZ-PDF equation. In particular, the approximation obtained by retaining only the first two cumulants is known as *Born approximation* in quantum field theory [17]. We remark that from the point of view of perturbation theory, the convolutionless form (22) has distinctive advantages over the usual convolution form (11). In particular, in the latter case a certain amount of rearrangement is necessary to obtain an expression which is correct up to a certain order in the coupling parameter [127].

Beyond Perturbation

Several attempts have been made to approximate MZ equations beyond closures based on perturbation analysis. For example, Chorin [27; 25; 24], Stinis [121; 120] and Chertok [20] proposed various models - such the t-model or the modified t model - for dimension reduction of autonomous dynamical systems in situations where there is no clear separation of scales between the resolved and the unresolved dynamics.

Another widely used closure approximation is based on the assumption that the distribution of the quantity of interest has a specific form, e.g., approximately Gaussian. This assumption can be justified in some cases on the basis of mixing, high-dimensionality and chaos. For example, the marginal densities of the Lorenz-96 system (9) are approximately Gaussian (see figure 4). In these cases, a Gaussian closure can be

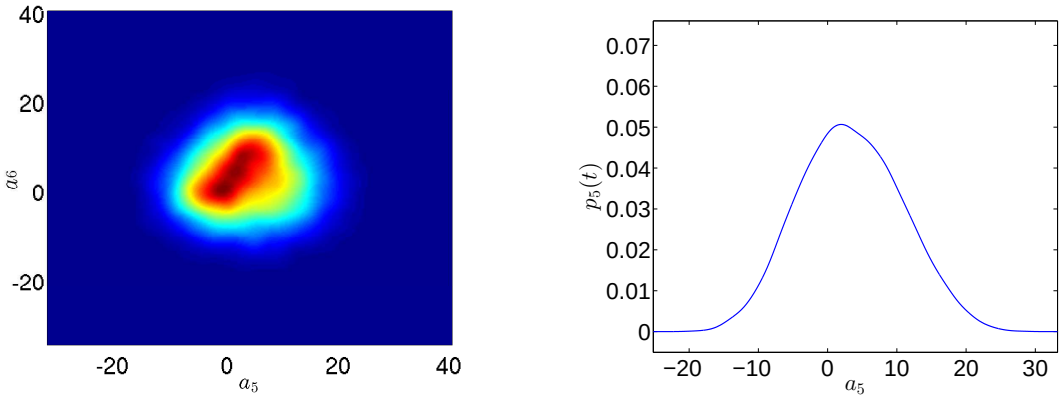

Fig. 4. Lorenz-96 system. Joint PDFs of different phase variables at time $t = 100$. Setting $c = 20$ in (9) yields a chaotic dynamics. In this case it can be shown that the joint PDF that solves Eq. (3) goes to a fractal attractor with Hausdorff dimension 34.5 [70]. However, the reduced-order PDFs are approximately Gaussian. This can be justified on the basis of chaos and multi-dimensional integration (6).

used to represent the PDF of the quantity of interest. Alternative methods rely, e.g, on maximum entropy closures [129; 61; 100; 63], and functional renormalization [121; 5], and *renormalized perturbation series* ([88], Ch. 5). The key idea is to use methods of many body-theory to generalize traditional perturbation series to the case of strong interactions [86]. These approaches have been used extensively in turbulence theory [88; 50].

A different technique to compute memory and the initial condition terms appearing in the Mori-Zwanzig equation relies on sampling, e.g., few realizations of the full dynamical system (1). In particular, one can leverage on implicit sampling techniques [26] and PDF estimates to construct a hybrid approach in which the memory and the initial condition terms in the MZ equation are computed on-the-fly based on both samples with an approximate MZ equation. In this way, one can compensate for the loss of accuracy associated with the approximation of the MZ equation with few samples of the full dynamical system. A closely related approach is to estimate the expansion coefficients of the effective propagator (subsequent section) by using samples

of the full dynamical system (1), and retain only the coefficients larger than a certain threshold.

Effective Propagators

Let us consider a dynamical system in the form (1) with time-independent f, i.e., an autonomous system. The formal solution to the joint PDF equation (3) in this case can be expressed as

$$p(t) = e^{tL} p(0). \tag{28}$$

If the initial state $p(0)$ is separable, i.e., if $p(0) = p_a(0)p_b(0)$ (where a and b are the relevant and irrelevant phase space coordinates), then the exact evolution of the relevant part of the PDF is given by

$$p_a(t) = \left\langle e^{tL} \right\rangle p_a(0), \tag{29}$$

where $\langle \cdot \rangle$ is an average with respect to the PDF $p_b(0)$. For example, the exact evolution of the PDF of the first component of the Lorentz-96 system (9) is given by

$$p_1(a_1, t) = \left(\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{tL} p_2(a_2, 0) \cdots p_n(a_n, 0) da_2 \cdots da_n \right) p_1(a_1, 0), \tag{30}$$

where L, in this case, is

$$L = -nI - \sum_{i=1}^{n} \left[(a_{i+1} - a_{i-2})\, a_{i-1} + a_i + c \right] \frac{\partial}{\partial a_i}. \tag{31}$$

The linear operator $\left\langle e^{tL} \right\rangle$ appearing in (29) is known as *relaxation operator* [75] or *effective propagator* [64; 88] of the reduced-order dynamics. Such propagator is no longer a semigroup as $\left\langle e^{(t+s)L} \right\rangle \neq \left\langle e^{tL} \right\rangle \left\langle e^{sL} \right\rangle$, i.e., the evolution of $p_a(t)$ is non-Markovian. This reflects the memory effect induced in the reduced-order dynamics when we integrate out the phase variables b. To compute the effective propagator we need to resort to approximations. For example, we could expand it in a power series [71; 35] as

$$\left\langle e^{tL} \right\rangle = I + \sum_{k=1}^{\infty} \frac{t^k}{k!} \left\langle L^k \right\rangle . \tag{32}$$

This expression shows that the dynamics of $p_a(t)$ is fully determined by the moments of the operator L relative to the joint distribution of the irrelevant phase variables. In particular, the kth-order moment $\left\langle L^k \right\rangle$ governing the dynamics of $p_1(a_1, t)$ in the Lorenz-96 system (30) is a linear differential operator in a_1 involving derivatives up to order k, i.e.,

$$\left\langle L^k \right\rangle = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \underbrace{L \cdots L}_{k \text{ times}} p_2(a_2, 0) \cdots p_n(a_n, 0) da_2 \cdots da_n \tag{33}$$

$$= \sum_{j=0}^{k} \alpha_j^{(k)}(a_1) \frac{\partial^j}{\partial a_1^j}. \tag{34}$$

The coefficients $\alpha_j^{(k)}$ can be calculated by substituting (31) into (33) and performing all integrations. This is a cumbersome calculation, but in principle it can be carried on and yields exact results. The problem is that truncating moment expansions such as (32) to any finite order usually yields results of poor accuracy. This is because we may be discarding secular terms growing like t^k, if the norm of $\left\langle L^k \right\rangle$ does not decay rapidly enough. A classical approach to overcome these limitation is to use operator cumulants [56; 75; 74; 65; 67]. For autonomous dynamical systems, we have the exact formula (see, e.g., [4])

$$\left\langle e^{tL} \right\rangle = e^{\left\langle e^{tL} - I \right\rangle_c}, \tag{35}$$

where $\langle \cdot \rangle_c$ here denotes a cumulant average, e.g.,

$$\langle L \rangle_c = \langle L \rangle , \qquad \left\langle L^2 \right\rangle_c = \left\langle L^2 \right\rangle - \langle L \rangle^2 , \qquad \cdots . \tag{36}$$

Following Kubo [75; 74], we emphasize that many different types of operator cumulants can be defined. Disregarding for, the moment, the specific *prescription* we use to construct such operator cumulants (see [75; 56]), let us differentiate (29) with respect to time and take (35) into account. This yields the following exact reduced-order PDF equation

$$\frac{\partial p_a(t)}{\partial t} = \left(\langle L \rangle_c + \sum_{k=2}^{\infty} \frac{t^{k-1}}{(k-1)!} \left\langle L^k \right\rangle_c \right) p_a(t), \tag{37}$$

which is completely equivalent to the MZ-PDF equation (22). Any truncation of the series expansion in (37) yields an approximated equation whose specific form depends on the way we define the cumulant average $\langle \cdot \rangle_c$. For example, we can get expansions in terms of *Kubo-Van Kampen*, *Waldenfels* or *Speicher* operator cumulants (see the Appendix of [137] or [56; 98]). The choice of the most appropriate operator cumulant expansion is problem-dependent.

Other methods to compute approximations to the effective propagator $\left\langle e^{tL} \right\rangle$ rely on functional renormalization, in particular on *renormalized perturbation series* ([88], Ch. 5). The key idea of these approaches is to use methods of many body-theory to generalize traditional perturbation series to the case of strong interactions. Formal treatment of this subject, along with the introduction of diagrammatic representations can be found in [88; 5]. If $p_a(t)$ involves q phase variables $(a_1, ..., a_q)$ then each $\left\langle L^k \right\rangle_c$ is a linear operator of order k involving a linear combination of generators $\partial^j / \partial a_k^j$ in the form

$$\left\langle L^k \right\rangle_c = \sum_{i_1,...,i_q=0}^{k} \beta^{(k)}_{i_1 \cdots i_q}(a_1, ..., a_q) \frac{\partial^{i_1+\cdots+i_q}}{\partial a_1^{i_1} \cdots \partial a_q^{i_q}}. \tag{38}$$

A substitution of this series expansion into Eq. (37) immediately suggests that the exact evolution of the reduced order PDF $p_a(t)$ is governed, in general, by a linear PDE involving derivatives of *infinite-order* in the phase variables $(a_1, ..., a_q)$. All coefficients $\beta^{(k)}_{i_1 \cdots i_q}(a_1, ..., a_q)$ appearing in (38) can be expressed in terms of integrals of polynomial functions of f_i (see equation (1)). However, computing such coefficients at all orders is not trivial nor practical. On the other hand, determining an approximated advection-diffusion form of (37) is possible, simply by taking into account those coefficients leading to second-order derivatives in the phase variables. This can be achieved in a systematic way by truncating the series (38) to derivatives of second-order and computing the corresponding coefficients.

Operator Splitting and Series Expansions

Let us consider an autonomous dynamical system evolving from a random initial state. The propagator $U(t,t_0) = e^{(t-t_0)L}$ forms a semigroup and therefore it can be split as

$$U(t_n,t_0) = U(t_n,t_{n-1}) \cdots U(t_2,t_1)U(t_1,t_0). \tag{39}$$

Each operator $U(t_i,t_{i-1})$ (short-time propagator) can be then approximated according to an appropriate decomposition formula [123; 124; 151; 10]. In particular, if L is given by (3) and if $\Delta t = |t_i - t_{i-1}|$ is small, then one can use the following first-order approximation

$$\exp\left[-\Delta t\left(\sum_{i=1}^{n}\frac{\partial f_i}{\partial a_i} + f_i\frac{\partial}{\partial a_i}\right)\right] \simeq \exp\left[-\Delta t\sum_{i=1}^{n}\frac{\partial f_i}{\partial a_i}\right]\prod_{k=1}^{n}\exp\left[-\Delta t f_k\frac{\partial}{\partial a_k}\right]. \tag{40}$$

This allows us *to split the joint PDF equation (3) into a system of PDF equations*. This approach is quite standard in numerical methods to solve linear PDEs in which the generator of the semigroup can be represented as a superimposition of linear operators. The error estimate for the decomposition formula (40) is given in [123; 125]. Higher-order formulas such as Lie-Trotter, Suzuki, and related Backer-Campbell-Hausdorff formulas can be constructed as well. The literature on this subject is very rich, e.g. [9; 15; 128; 149; 152; 123].

A somewhat related approach relies on approximating the exponential semigroup e^{tL} in terms of operator polynomials, e.g., the *Faber polynomials* F_k [104]. In this case, the exact evolution of the PDF can be expressed as

$$p_a(t) = \sum_{k=0}^{N}\psi_k(t)\Phi_k(a), \qquad \text{where} \qquad \Phi_k(a) = \langle F_k(L)\rangle\, p_a(0). \tag{41}$$

In particular, if F_k are generated by elliptic conformal mappings then they satisfy a three-term recurrence in the form

$$F_{k+1}(L) = (L - c_0)F_k(L) - c_1F_{k-1}(L), \qquad F_0(L) = I, \tag{42}$$

which yields an *unclosed* three-term recurrence for the *modes* Φ_k

$$\Phi_{k+1}(a) = \langle LF_k(L)\rangle\, p_a(0) - c_0\Phi_k(a) - c_1\Phi_{k-1}(a), \qquad \Phi_0(a) = 1. \tag{43}$$

In some cases, the operator averages $\langle L^n\rangle$ appearing in $\langle LF_k(L)\rangle$ can be reduced to one-dimensional integrals. This happens, in particular, if the initial $p(0)$ is separable, and if the functions f_k appearing in (1) are separable as well. Although this might seem a severe restriction, it is actually satisfied by many systems including Lorentz-96 [80], Kraichnan-Orszag [107], and the semi-discrete form of SPDEs with polynomial-type nonlinearities (e.g., viscous Burgers and Navier-Stokes equations).

Algorithms and Solvers

MZ-PDF equations are a particular class of probability density function equations involving memory and initial condition terms. Computing the numerical solution to a probability density function equation is, in general, a very challenging task that involves several problems of different nature. In particular,

High-Dimensionality: PDF equations describing realistic physical systems usually involve many phase variables. For example, the Fokker-Planck equation of classical statistical mechanics yields a joint probability density function in n phase variables, where n is the dimension of the underlying dynamical system, plus time.

Multiple Scales: PDF equations may involve multiple scales in space and time, which could be hardly accessible by conventional numerical methods. For example, the joint PDF equation (3) is a hyperbolic conservation law whose solution is purely advected (with no diffusion) by the compressible flow G. This can easily yield mixing, fractal attractors, and all sorts of complex dynamics (see Fig. 1).

Lack of Regularity: The solution to a PDF equation is, in general, a distribution [69]. For example, it could be a multivariate Dirac delta function, a function with shock-type

discontinuities [23], or even a fractal object. From a numerical viewpoint, resolving such distributions is not trivial although in some cases it can be done by taking integral transformations or projections [157]. An additional numerical difficulty inherent to the simulation of PDF equations arises due to the fact that the solution could be compactly supported over disjoint domains. This obviously requires the development of appropriate numerical techniques such as adaptive discontinuous Galerkin methods [21; 28; 114].

Conservation Properties: There are several properties of the solution to a PDF equation that must be preserved in time. The most obvious one is mass, i.e., the solution always integrates to one. Another property that must be preserved is the positivity of the joint PDF, and the fact that a partial marginalization of a joint PDF still yields a PDF.

Long-Term Integration: The flow map defined by nonlinear dynamical systems can yield large deformations, stretching and folding of the phase space. As a consequence, numerical schemes for kinetic equations associated with such systems will generally loose accuracy in time.

Over the years, many different methods have been proposed to address these issues, with the most efficient ones being problem-dependent. For example, a widely used method in statistical fluid mechanics is the particle/mesh method [111; 112; 110; 96], which is based directly on stochastic Lagrangian models. Other methods make use of stochastic fields [130] or direct quadrature of moments [48]. In the case of Boltzmann equation, there is a very rich literature. Both probabilistic approaches such as direct simulation Monte Carlo [8; 117], as well as deterministic methods, e.g., discontinuous Galerkin and spectral methods [40; 18; 19], have been proposed to compute the solution. Probabilistic methods such as direct simulation Monte Carlo are extensively used because of their very low computational cost compared to finite-volumes, finite-differences or spectral methods, especially in the multi-dimensional case. How-

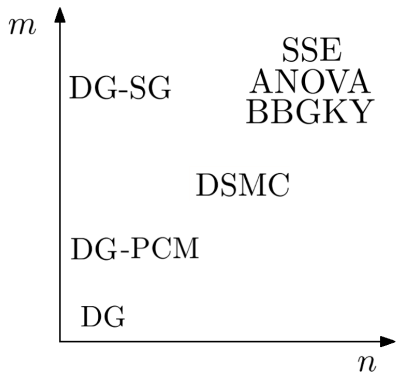

Fig. 5. Range of applicability of numerical methods for solving PDF equations as a function of the number of phase variables n and the number parameters m appearing in the equation. Shown are: Separated series expansion methods (SSE), BBGKY closures, high-dimensional model representations (ANOVA), adaptive discontinuous Galerkin methods (DG) combined with sparse grids (SG) or tensor product probabilistic collocation (PCM), direct simulation Monte Carlo (DSMC).

ever, Monte Carlo usually yields poorly accurate and fluctuating solutions, which need to be post-processed appropriately, for example through variance reduction techniques. We refer to Dimarco and Pareschi [32] for a recent review.

In our previous work [21], we addressed the lack of regularity and high-dimensionality (in the space of parameters) of kinetic equations by using adaptive discontinuous Galerkin methods [29; 115] combined with sparse probabilistic collocation. Specifically, the phase variables of the system were discretized by using spectral elements on an adaptive non-conforming grid that tracks the support of the PDF in time, while the parametric dependence of the solution was handled by using sparse grids. More recently, we proposed and validated new classes of algorithms addressing the high-dimensional challenge in PDF equations [22]. These algorithms rely on separated series expansions, high dimensional model representations and BBGKY hierarchies. Their range of applicability is sketched in Fig. 5 as a function of the number of phase variables n and the number of parameters m appearing in the PDF equation (see also Eq. (1)).

The numerical treatment of MZ-PDF equations is even more challenging than classical PDF equations, due to the complexity of the memory and the initial condition terms. Such terms involve the projected part of the full orthogonal dynamics, which is represented by an exponential operator of very high dimension. Computing the solution to MZ-PDF equations, therefore, heavily relies on the approximation of memory and initial condition terms, e.g., in terms of operator cumulants [137; 23], approximate exponential matrices [2; 3; 89] or samples of the full dynamical system [24]. Developing new algorithms to compute the solution to MZ-PDF equations is a matter for future research.

Applications

In this section we illustrate the application of the the Mori-Zwanzig formulation to some well-know stochastic systems.

Stochastic Resonance Driven by Colored Noise

Let us consider a nonlinear dynamical system subject to a weak deterministic periodic signal and additive colored random noise. As is well known, in some cases, e.g., in bistable systems, the cooperation between noise and signal can yield a phenomenon known as *stochastic resonance* [6; 83; 148; 105], namely random noise can enhance significantly the transmission of the weak periodic signal. The mechanism that makes this possible is explained in Fig. 6, with reference to the system

$$\begin{cases} \dfrac{dx(t)}{dt} = \dfrac{2\mu x - 2\nu x^3 - \nu x^5}{2(1+x^2)^2} + \sigma f(t;\xi) + \epsilon\cos(\Omega t) \\ x(0) = x_0(\omega) \end{cases} . \tag{44}$$

Here $\xi \in \mathbb{R}^m$ is a vector of uncorrelated Gaussian random variables while $x_0 \in \mathbb{R}$ is a Gaussian initial state. Also, the random noise $f(t;\xi)$ is assumed to be a zero-mean

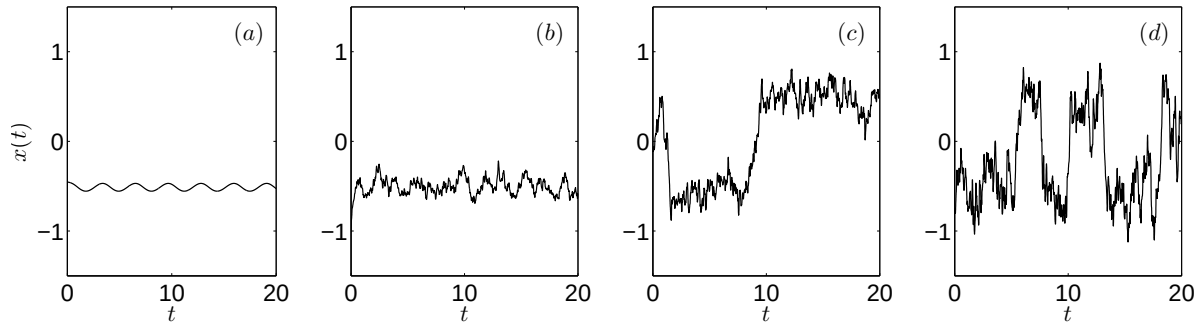

Fig. 6. Stochastic resonance. We study the system (44) with parameters $\mu = 10$, $\nu = 3$, $\Omega = 2$, $\epsilon = 0.2$ subject to weakly colored random noise ($\tau = 0.01$) of different amplitudes: (a) $\sigma = 0$; (b) $\sigma = 0.2$; (c) $\sigma = 0.4$; (d) $\sigma = 0.8$. Each figure shows only one solution sample. At low noise levels the average residence time in the two states is much longer than the driving period. However, if we increase the noise level to $\sigma = 0.8$ (Fig. (d)), then we observe almost periodic transitions between the two meta-stable states. In most cases, we have a jump from one state to the other and back again approximately once per modulation period. (Adapted from [137]).

Gaussian process with exponential covariance function

$$C(t,s) = \frac{1}{2\tau} e^{-|t-s|/\tau} \tag{45}$$

and finite correlation time τ.

Mori-Zwanzig Equation

The exact evolution equation for the PDF of $x(t)$ can be obtained by applying the convolutionless projection operator method described in previous sections. Such equation is a linear partial differential equation of *infinite-order* in the phase variable a. If we consider a second-order approximation, i.e., if we expand propagator of p_x in terms of cumulant operators and truncate the expansion at the second order, then we obtain

$$\frac{\partial p_x}{\partial t} = L_0 p_x - \epsilon \cos(\Omega t) \frac{\partial p_x}{\partial a} + \sigma^2 \left[\int_0^t C(t,s) \frac{\partial}{\partial a} e^{(t-s)L_0} \frac{\partial}{\partial a} e^{(s-t)L_0} ds \right] p_x, \tag{46}$$

where

$$L_0 = \frac{\partial}{\partial a} \left(\frac{2\mu a - 2\nu a^3 - \nu a^5}{2(1+a^2)^2} \right) I + \left(\frac{2\mu a - 2\nu a^3 - \nu a^5}{2(1+a^2)^2} \right) \frac{\partial}{\partial a}. \tag{47}$$

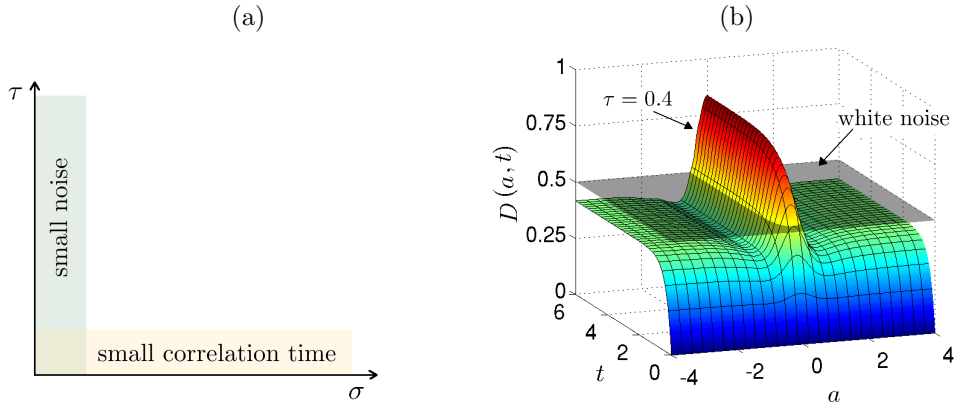

Fig. 7. Stochastic resonance. Range of validity of the MZ-PDF equation (46) as a function of the noise amplitude σ and correlation time τ (Fig. (a)). Effective diffusion coefficient $D(a,t)$ (see Eq. (48)) corresponding to exponentially correlated Gaussian noises (Fig. (b)). (Adapted from [137]).

The rationale behind this approximation is that higher-order cumulants can be neglected [37; 38]. This happens, in particular, if both ϵ and σ are small. Faetti et. *al.* [37; 38] have shown that for $\epsilon = 0$ the correction due to the fourth-order cumulants are of order $\sigma\tau^2$ for Gaussian noise and order $\sigma\tau$ for other noises. Thus, (46) holds true either for small ϵ and σ and arbitrary correlation time τ or for small ϵ and τ and arbitrary noise amplitude σ (see Fig. 7). It can be shown (see, e.g., [137; 94]) that (46) is equivalent to the following *advection-diffusion equation*

$$\frac{\partial p_x}{\partial t} = L_0 p_x - \varepsilon \cos(\Omega t)\frac{\partial p_x}{\partial a} + \sigma^2 \frac{\partial^2}{\partial a^2}\left(D(a,t)p_x\right), \tag{48}$$

where the effective diffusion coefficient $D(a,t)$ depends on the type of noise. Note that if the correlation time τ goes to zero (white-noise limit), then Eq. (46), with $C(t,s)$ defined in (45), consistently reduces to the classical Fokker-Planck equation. The proof is simple, and it relies on the limits

$$\lim_{\tau\to 0}\int_0^t \frac{1}{2\tau}e^{-s/\tau}ds = \frac{1}{2}, \qquad \lim_{\tau\to 0}\int_0^t \frac{1}{2\tau}e^{-s/\tau}s^k ds = 0, \qquad k \in \mathbb{N}. \tag{49}$$

These equations allow us to conclude that

$$\lim_{\tau\to 0}\int_0^t \frac{1}{2\tau}e^{-s/\tau}\frac{\partial}{\partial a}e^{sL_0}\frac{\partial}{\partial a}e^{-sL_0}ds = \lim_{\tau\to 0}\left[\int_0^t \frac{1}{2\tau}e^{-s/\tau}ds\right]\frac{\partial^2}{\partial a^2} = \frac{1}{2}\frac{\partial^2}{\partial a^2}, \tag{50}$$

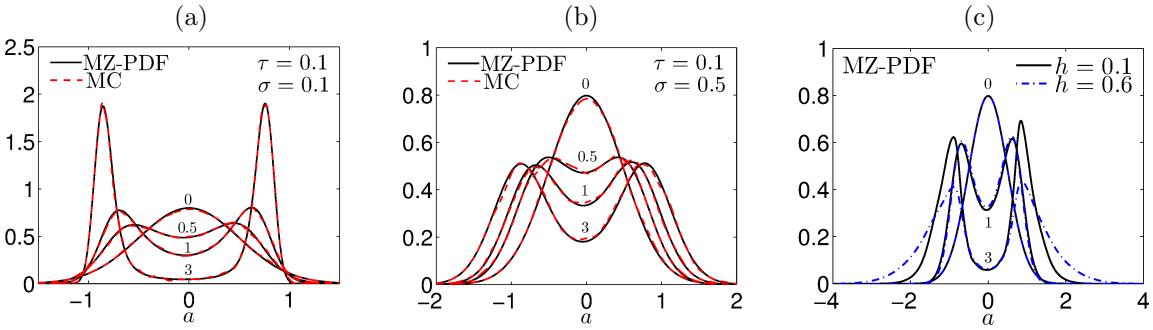

Fig. 8. Stochastic resonance. Time snapshots of the PDF of $x(t)$ as predicted by Eq. (46) (continuous lines) and MC simulation (10^5 samples) (dashed lines). The Gaussian process $f(t;\xi)$ in (44) is exponentially with small correlation time τ (Fig. (a) and (b)). Note that the Karhunen-Loève expansion of such noise requires 280 Gaussian random variables to achieve 99% of the correlation energy in the time interval $[0,3]$. We also show the PDF dynamics corresponding to fractional Brownian motion of small amplitude and different Hurst indices (Fig. (c)). (Adapted from [137]).

i.e., for $\tau \to 0$ Eq. (46) reduces to the Fokker-Planck equation

$$\frac{\partial p_x}{\partial t} = L_0 p_x - \epsilon \cos(\Omega t)\frac{\partial p_x}{\partial a} + \frac{\sigma^2}{2}\frac{\partial^2 p_x}{\partial a^2}. \tag{51}$$

Next, we study the transient dynamics of the one-time PDF of the solution $x(t)$ within the period $T = 3$. To this end, we consider the following set of parameters $\mu = 1$, $\nu = 1$, $\Omega = 10$, $\epsilon = 0.5$, leading to a slow relaxation to statistical equilibrium. This allows us to study the transient of the PDF more carefully, and compare the results with Monte Carlo (MC). This is done in Fig. 8, where it is seen that for small σ the random forcing term in (44) does not influence significantly the dynamics and therefore the PDF of $x(t)$ is mainly advected by the operator L_0. Note that the PDF tends to accumulate around the meta-stable equilibrium states $\pm\sqrt{\sqrt{3}-1}$. For larger σ the probability of switching between the meta-stable states increases and therefore the strong bi-modality observed in Fig. 8 (left) is attenuated.

Fractional Brownian Motion, Levy, and Other Noises

There exist a close connection between the statistical properties of the random noise and the structure of the MZ-PDF equation for the response variables of the system. In particular, it has been recently shown, e.g. in [76], that the PDF of the solution to the Langevin equation driven by Levy flights satisfies a *fractional* Fokker-Plank equation. Such equation can be easily derived by using the Mori-Zwanzig projection operator framework, which represents therefore a very general tool to exploit the relation between noise and reduced-order PDF equations. For example, let us consider the non-stationary covariance function of *fractional Brownian motion*

$$C(t,s) = \frac{1}{2}\left(|t|^{2h} + |s|^{2h} - |t-s|^{2h}\right), \qquad 0 < h < 1, \qquad t, s > 0 \tag{52}$$

which reduces to the covariance function of standard Levy noise for $h = 1/2$, i.e., $C_{Levy}(t,s) = \min\{t,s\}$. A substitution of (52) into (46) yields an equation for the PDF of the solution to the system (1) driven by fractional Brownian motion of *small amplitude*. As is well known, such noise can trigger either sub-diffusion or super-diffusion in the PDF dynamics.

Stochastic Advection-Reaction

Let us consider the advection-reaction equation for a scalar concentration field

$$\frac{\partial u}{\partial t} + V(x) \cdot \nabla u = \left[\kappa_0(x) + \sigma\kappa_1(x;\xi)\right] R(u), \qquad \xi \in \mathbb{R}^m, \tag{53}$$

where $V(x)$ is a divergence-free (deterministic) advection velocity field, $R(u)$ is a nonlinear reaction term and $\kappa_1(x;\xi)$ is a zero-mean random perturbation in the reaction rate $\kappa_0(x)$. In Fig. 9 we plot few samples of the concentration field solving (53) in one spatial dimension, for different realizations of the random reaction rate and the random initial condition. In [142; 136] we have studied Eq. (53) by using the response-excitation

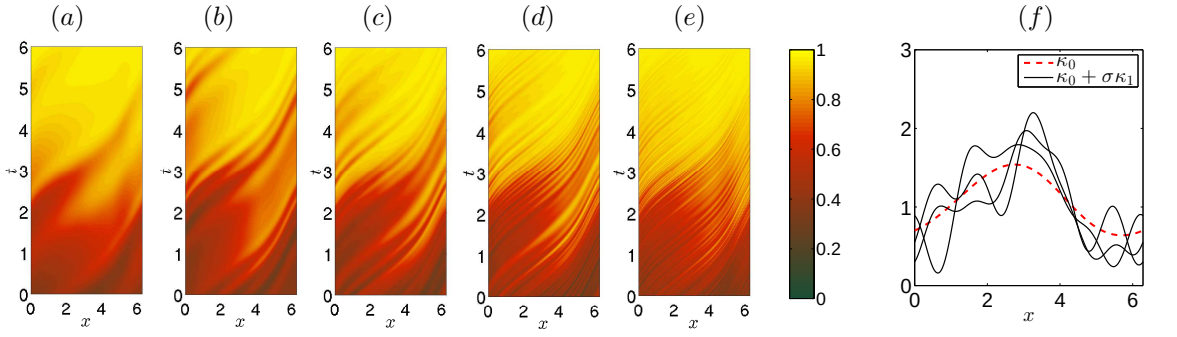

Fig. 9. Stochastic advection-reaction. Samples of the concentration field solving (53) in one spatial dimension for periodic boundary conditions and different realizations of the random initial condition and the random reaction rate. The correlation length of the random initial condition decreases from (a) to (e). In (f) we plot few realizations of the random reaction rate ($\sigma = 0.3$). (Adapted from [137]).

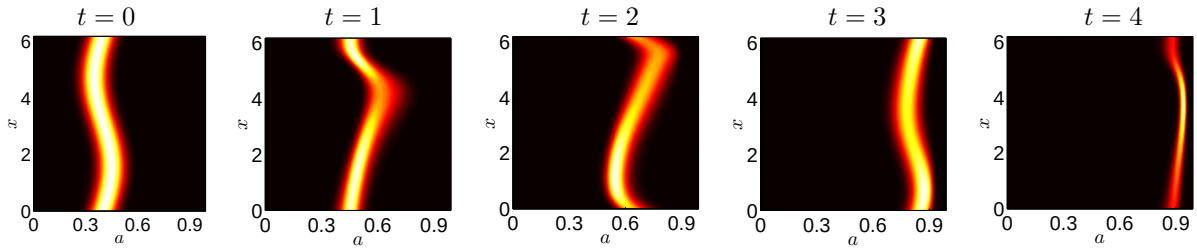

Fig. 10. Stochastic advection-reaction. Time snapshots of the concentration PDF predicted by the MZ-PDF equation (54). (Adapted from [137]).

PDF method as well as the large-eddy-diffusivity (LED) closure [126]. Here we consider a different approach based on the MZ-PDF equation [137] . To this end, we assume that σ is reasonably small and that the concentration field u is independent of ξ at initial time, i.e., that the initial joint PDF of the system has the form $p(0) = p_u(0)p_\xi$. In these hypotheses, we obtain the following second-order approximation to the MZ-PDF equation

$$\frac{\partial p_u(t)}{\partial t} = L_0 p_u(t) + \sigma^2 \left[\int_0^t \left\langle \kappa_1 e^{sL_0} \kappa_1 \right\rangle e^{-sL_0} ds \right] F^2 p_u(t), \tag{54}$$

where the average $\langle \cdot \rangle$ is relative to the joint PDF of ξ and

$$L_0 = -\kappa_0(x)F - V(x) \cdot \nabla, \qquad F = \frac{\partial R(a)}{\partial a} + R(a)\frac{\partial}{\partial a}. \tag{55}$$

Equation (54) is linear, but it involves derivatives of infinite-order in both variables x and a. Such derivatives come from the exponential operators e^{sL_0} within the time

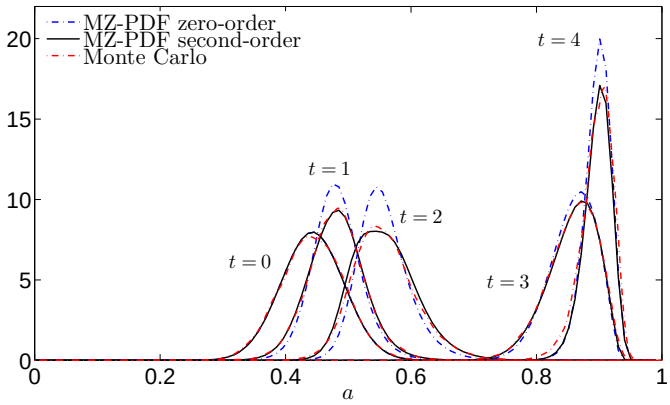

Fig. 11. Stochastic advection-reaction. Comparison between the MZ-PDF solution at $x = 1$ and a non-parametric kernel density estimation [12] of the PDF based on 10000 MC solution samples. The zero-order approximation is obtained by neglecting the second-order term in σ in Eq. (54). (Adapted from [137]).

convolution term. Note that such convolution can be also expressed as a functional derivative [134] of the exponential operator along $\kappa_1(x)$, by using an identity of Feynman (see [39], Eq. (6) or [152]). In a finite-dimensional setting, these quantities can be computed by using efficient numerical algorithms, e.g., based on scaling-squaring methods and Padé approximants [2; 3; 89]. In Fig. 10 we plot the time snapshots of the PDF of the concentration field as predicted by the MZ-PDF equation (54). The comparison between such PDF and a Monte-Carlo solution is done in Fig. 11. It is seen that in this case the second-order operator cumulant approximation provides accurate results for a quite large degree of perturbation (see Fig. 9(f)).

Stochastic Burgers Equation

The Mori-Zwanzig formulation can be applied also to the Burgers equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \sigma f(x,t;\omega) \tag{56}$$

to formally integrate out the random forcing term. This yield the following equation (second-order approximation) for the one-point one-time PDF of the velocity field (see

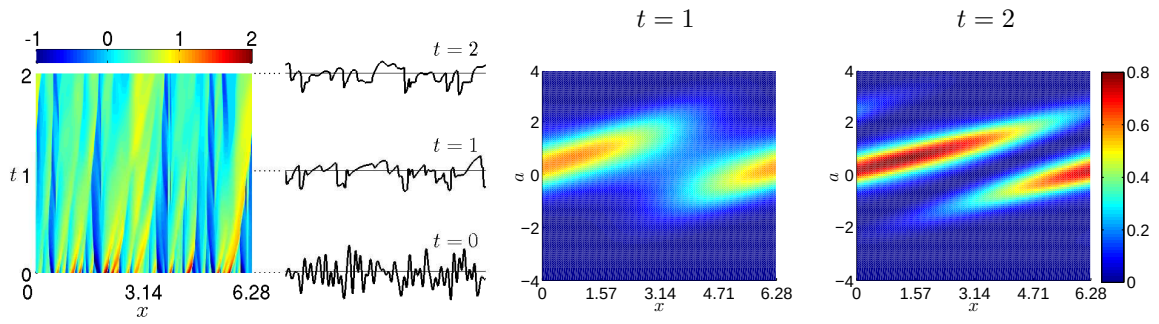

Fig. 12. Stochastic Burgers equation. One realization of the velocity field computed by using adaptive discontinuous Galerkin methods (left). Time snapshots of the one-point PDF obtained by solving the MZ-PDF equation (57). Adapted from [23])

[23])

$$\frac{\partial p_u(t)}{\partial t} = L_0 p_u(t) + \sigma \langle f(x,t) \rangle \frac{\partial p_u(t)}{\partial a} + \sigma^2 \left[\int_0^t \left\langle f(x,t) \frac{\partial}{\partial a} e^{(t-s)L_0} f(x,s) \right\rangle \frac{\partial}{\partial a} e^{-(t-s)L_0} ds \right] p_u(t), \tag{57}$$

where L_0 is given by

$$L_0 = -\int_{-\infty}^{a} da \frac{\partial}{\partial x} - a \frac{\partial}{\partial x}. \tag{58}$$

In Fig. 13 we compare the PDF dynamics obtained by solving Eq. (57) with Monte Carlo simulation. It is seen that, as we increase the amplitude σ of the forcing, the second-order approximation (57) loses accuracy and higher-order corrections have to be included.

Coarse-Grained Models of Particle Systems

Particle systems are often used in models of system biology and soft matter physics to simulate and understand large-scale effects based on microscopic first principles. The computability of such systems depends critically on the number of particles and the interaction potentials. Full molecular dynamics (MD) simulations can be performed for particle systems with $\mathcal{O}(10^{13})$ particles. However, such "hero" simulations require hundred of thousands of computer cores and significant time and data processing to be successfully completed. This motivates the use of coarse-graining techniques, such

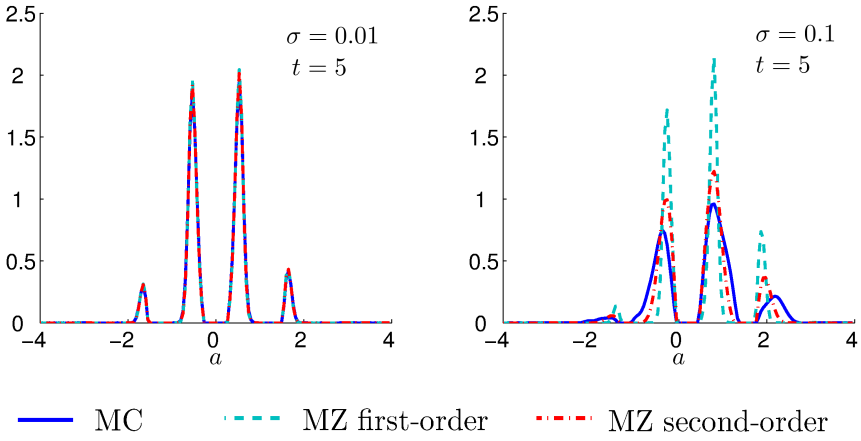

Fig. 13. Stochastic Burgers equation. One-point PDF of the velocity field at $x = \pi$ for exponentially correlated, homogeneous (in space) random forcing processes with correlation time 0.01 and amplitude $\sigma = 0.01$ and $\sigma = 0.1$ (second row). Shown are results obtained from MC, and from two different truncations of the MZ-PDF equation (57). (Adapted from [23]).

as dissipative particle dynamics (DPD) [99], for particle systems to compute macroscopic/mesoscopic observables at a reasonable computational cost. Among different approaches, the Mori-Zwanzig formulation [62; 119] has proved to be effective in achieving this goal [78; 1; 59]. The key idea is shown in Fig. 14, where a star polymer described atomistically is coarse-grained to bigger particles - the MZ-DPD particles - by following the procedure sketched in Fig. 3 for a star polymer. The calculation of the solution to the MZ-DPD system, e.g., Eq. (14), relies on approximations. In particular, the memory term plays an important role in the dynamics of the coarse-grained system, and this role becomes more relevant as we increase the coarse-graining level [158; 78]. In Fig. 14 we compare the velocity auto-correlation function obtained from molecular dynamics simulations (MD) and the coarse-grained MZ-DPD system.

Conclusions

In this chapter we discussed how to perform the contraction of state variables in non-equilibrium stochastic dynamical systems by using the Mori-Zwanzig projection opera-

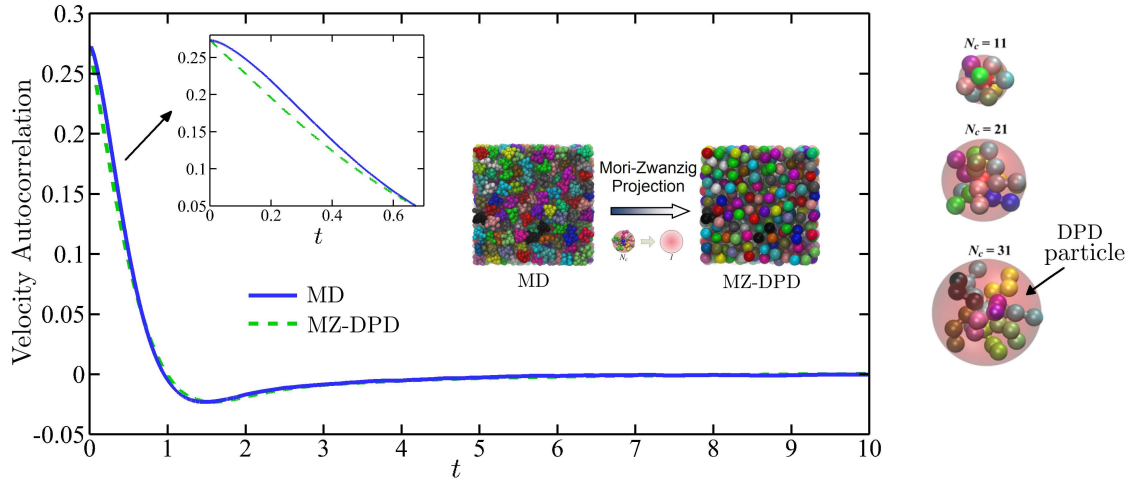

Fig. 14. Coarse-grained model of a particle system. Comparison between the velocity auto-correlation function obtained from molecular dynamics simulation (MD) and Mori-Zwanzig dissipative particle-dynamics (MZ-DPD). (Courtesy of Dr. Zhen Li, Brown University (unpublished)).

tor method and the effective propagator approaches. Both techniques yield exact equations of motion for quantities of interest in high-dimensional systems, e.g., functionals of the solution to systems of stochastic ordinary and partial differential equations. Examples of such functionals are the position and momentum of clusters of particles (MZ-DPD methods), the series expansion of the solution to a SPDE, or the turbulent viscosity in the inertial range of fully developed turbulence. One of the main advantages in developing such exact equations is that they allow us to avoid integrating the full (high-dimensional) stochastic dynamical system and solve directly for the quantities of interest, thus reducing the computational cost significantly. In principle, this can break the curse of dimensionality in numerical simulations of SODEs and SPDEs at the price of solving complex integro-differential equations. Computing the solution to MZ equations relies on approximations and appropriate numerical schemes. Over the years many different techniques have been proposed for this scope, with the most efficient ones being problem-dependent. We discussed classical perturbation methods such as truncated operator cumulant expansions, as well as more recent approaches, e.g., based on orthogonal expansions of memory kernels, renormalized perturbation theory,

sampling techniques, and maximum entropy principles. There is no general recipe to effectively approximate MZ equations for systems in which the relevant and the irrelevant phase variables have similar dynamical properties and order of magnitude. This situation arises very often when dealing with the problem of eliminating macroscopic phase variables, and it should be approached on a case-by-case basis.

Cross-references

PDF Methods for Uncertainty Quantification; Polynomial Chaos: Modeling, Estimation, and Approximation; Low-rank and Sparse Tensor Methods for High-dimensional Stochastic Problems; Hierarchical Models for Uncertainty Quantification: An Overview; Multiresolution Methods for Parametric Uncertainty Propagation; Random Vectors and Random Fields in High Dimension. Parametric Model-based Representation, Identification from Data, and Inverse Problems; Reduced Basis and Model Reduction for UQ; Sparse Collocation Methods for Stochastic Interpolation and Quadrature; Stochastic Collocation Methods: A Survey.

References

1. Akkermans RLC, Briels WJ (2000) Coarse-grained dynamics of one chain in a polymer melt. J Chem Phys 113(15):620–630
2. Al-Mohy AH, Higham NJ (2009) Computing the Fréchet derivative of the matrix exponential with an application to condition number estimation. SIAM J Matrix Anal Appl 30(4):1639–1657
3. Al-Mohy AH, Higham NJ (2011) Computing the action of the matrix exponential with an application to exponential integrators. SIAM J Sci Comput 33(2):488–511
4. Arai T, Goodman B (1967) Cumulant expansion and Wick theorem for spins. Application to the antiferromagnetic ground state. Phys Rev 155(2):514–527
5. Balescu R (1975) Equilibrium and non-equilibrium statistical mechanics. John Wiley & Sons

6. Benzi R, Sutera A, Vulpiani A (1981) The mechanism of stochastic resonance. J Phys A: Math Gen 14:L453–L457
7. Billings SA (2013) Nonlinear system identification: NARMAX methods in the time, frequency, and spatio-temporal domains. Wiley
8. Bird GA (1994) Molecular gas dynamics and direct numerical simulation of gas flows. Clarendon Press
9. Blanes S, Casas F, Oteo JA, Ros J (2009) The Magnus expansion and some of its applications. Physics Reports 470:151–238
10. Blanes S, Casas F, Murua A (2012) Splitting methods in the numerical integration of non-autonomous dynamical systems. RACSAM 106:49–66
11. Bonatto C, Gallas JAC, Ueda Y (2008) Chaotic phase similarities and recurrences in a damped-driven Duffing oscillator. Phys Rev E 77:026,217(1–5)
12. Botev ZI, Grotowski JF, Kroese DP (2010) Kernel density estimation via diffusion. Annals of Statistics 38(5):2916–2957
13. Breuer HP, Kappler B, Petruccione F (2001) The time-convolutionless projection operator technique in the quantum theory of dissipation and decoherence. Annals of Physics 291:36–70
14. Broer H, Simó C, Vitolo R (2002) Bifurcations and strange attractors in the Lorenz-84 climate model with seasonal forcing. Nonlinearity 15:1205–1267
15. Casas F (1996) Solutions of linear partial differential equations by Lie algebraic methods. J Comput Appl Math 76:159–170
16. Cercignani C, Gerasimenko UI, Petrina DY (eds) (1997) Many particle dynamics and kinetic equations, 1st edn. Kluwer Academic Publishers
17. Chaturvedi S, Shibata F (1979) Time-convolutionless projection operator formalism for elimination of fast variables. Applications to Brownian motion. Z Physik B 35:297–308
18. Cheng Y, Gamba IM, Majorana A, Shu CW (2009) A discontinuous Galerkin solver for Boltzmann-Poisson systems in nano devices. Computer Methods in Applied Mechanics and Engineering 198:3130–3150
19. Cheng Y, Gamba IM, Majorana A, Shu CW (2011) A brief survey of the discontinuous Galerkin method for the Boltzmann-Poisson equations. SEMA J 54:47–64
20. Chertock A, Gottlieb D, Solomonoff A (2008) Modified optimal prediction and its application to a particle method problem. J Sci Comput 37(2):189,201

21. Cho H, Venturi D, Karniadakis GE (2013) Adaptive discontinuous Galerkin method for response-excitation PDF equations. SIAM J Sci Comput 5(4):B890B911
22. Cho H, Venturi D, Karniadakis GE (2014) Numerical methods for high-dimensional probability density function equations. J Comput Phys Under Review
23. Cho H, Venturi D, Karniadakis GE (2014) Statistical analysis and simulation of random shocks in Burgers equation. Proc R Soc A 2171(470):1–21
24. Chorin A, Lu F (2015) A discrete approach to stochastic parametrization and dimensional reduction in nonlinear dynamics. arXiv:submit/1219662 pp 1–12
25. Chorin AJ, Stinis P (2006) Problem reduction, renormalization and memory. Comm App Math and Comp Sci 1(1):1–27
26. Chorin AJ, Tu X (2009) Implicit sampling for particle filters. PNAS 106(41):17,249–17,254
27. Chorin AJ, Hald OH, Kupferman R (2000) Optimal prediction and the Mori-Zwanzig representation of irreversible processes. Proc Natl Acad Sci USA 97(7):2968–2973
28. Cockburn B, Karniadakis GE, Shu CW (2000) Discontinuous Galerkin methods. Springer, vol. 11 of Lecture Notes in Computational Science and Engineering
29. Cockburn B, Karniadakis GE, Shu CW (2000) Discontinuous Galerkin methods. Springer, vol. 11 of Lecture Notes in Computational Science and Engineering
30. Darve E, Solomon J, Kia A (2009) Computing generalized Langevin equations and generalized Fokker-Planck equations. Proc Natl Acad Sci USA 106(27):10,884–10,889
31. Dekker H (1982) Correlation time expansion for multidimensional weakly non-Markovian Gaussian processes. Phys Lett A 90(1-2):26–30
32. Dimarco G, Paresci L (2014) Numerical methods for kinetic equations. Acta Numerica 23(4):369–520
33. Doostan A, Owhadi H (2011) A non-adapted sparse approximation of PDEs with stochastic inputs. J Comput Phys 230(8):3015–3034
34. Edwards SF (1964) The statistical dynamics of homogeneous turbulence. J Fluid Mech 18:239–273
35. Engel KJ, Nagel R (2000) One-parameter semigroups for linear evolution equations. Springer
36. Faetti S, Grigolini P (1987) Unitary point of view on the puzzling problem of nonlinear systems driven by colored noise. Phys Rev A 36(1):441–444

37. Faetti S, Fronzoni L, Grigolini P, Mannella R (1988) The projection operator approach to the Fokker-Planck equation. I. Colored Gaussian noise. J Stat Phys 52(3/4):951–978

38. Faetti S, Fronzoni L, Grigolini P, Palleschi V, Tropiano G (1988) The projection operator approach to the Fokker-Planck equation. II. Dichotomic and nonlinear Gaussian noise. J Stat Phys 52(3/4):979–1003

39. Feynman RP (1951) An operator calculus having applications in quantum electrodynamics. Phys Rev 84:108–128

40. Filbet F, Russo G (2003) High-order numerical methods for the space non-homogeneous Boltzmann equations. J Comput Phys 186:457–480

41. Foias C, Sell GR, Temam R (1988) Inertial manifolds for nonlinear evolutionary equations. Proc Natl Acad Sci USA 73(2):309–353

42. Foias C, Manley OP, Rosa R, Temam R (2001) Navier-Stokes equations and turbulence, 1st edn. Cambridge University Press

43. Foias C, Jolly MS, Manley OP, Rosa R (2002) Statistical estimates for the Navier-Stokes equations and Kraichnan theory of 2-D fully developed turbulence. J Stat Phys 108(3/4):591–646

44. Foo J, Karniadakis GE (2008) The multi-element probabilistic collocation method (ME-PCM): Error analysis and applications. J Comput Phys 227:9572–9595

45. Foo J, Karniadakis GE (2010) Multi-element probabilistic collocation method in high dimensions. J Comput Phys 229:1536–1557

46. Fox RF (1975) A generalized theory of multiplicative stochastic processes using cumulant techniques. J Math Phys 16(2):289–297

47. Fox RF (1986) Functional-calculus approach to stochastic differential equations. Phys Rev A 33(1):467–476

48. Fox RO (2003) Computational Models for Turbulent Reactive Flows. Cambridge University Press

49. Friedrich R, Daitche A, Kamps O, Lülff J, Voβkuhle M, Wilczek M (2012) The Lundgren-Monin-Novikov hierarchy: kinetic equations for turbulence. Comptes Rendus Physique 13(9-10):929–953

50. Frisch U (1995) Turbulence: the legacy of A. N. Kolmogorov. Cambridge University Press

51. Ghanem RG, Spanos PD (1998) Stochastic finite elements: a spectral approach. Springer-Verlag

52. Hänggi P (1978) Correlation functions and master equations of generalized (non-Markovian) Langevin equations. Z Physik B 31:407–416

53. Hänggi P (1978) On derivations and solutions of master equations and asymptotic representations. Z Physik B 30:85–95

54. Hänggi P (1985) The functional derivative and its use in the description of noisy dynamical systems. In: Pesquera L, Rodriguez M (eds) Stochastic processes applied to physics, World Scientific, pp 69–95

55. Hänggi P, Jung P (1995) Colored noise in dynamical systems. In: Prigogine I, Rice SA (eds) Advances in Chemical Physics: Volume 89, Wiley-Interscience, pp 239–326

56. Hegerfeldt GC, Schulze H (1988) Noncommutative cumulants for stochastic differential equations and for generalized Dyson series. J Stat Phys 51(3/4):691–710

57. Herring JR (1966) Self-consistent-field approach to nonstationary turbulence. Phys Fluids 9(11):2106–2110

58. Hesthaven JS, Gottlieb S, Gottlieb D (2007) Spectral methods for time-dependent problems. Cambridge Univ. Press

59. Hijón C, nol PE, Vanden-Eijnden E, Delgado-Buscalioni R (2010) Mori-Zwanzig formalism as a practical computational tool. Faraday Discuss 144:301–322

60. Hosokawa I (2006) Monin-Lundgren hierarchy versus the Hopf equation in the statistical theory of turbulence. Phys Rev E 73:067,301(1–4)

61. Hughes KH, Burghardt I (2012) Maximum-entropy closure of hydrodynamic moment hierarchies including correlations. J Chem Phys 136:214,109(1–18)

62. Izvekov S (2013) Microscopic derivation of particle-based coarse-grained dynamics. J Chem Phys 138:134,106(1–16)

63. Jaynes ET (2003) Probability theory: the logic of science. Cambridge University Press

64. Jensen RV (1981) Functional integral approach to classical statistical dynamics. J Stat Phys 25(2):183–210

65. Kampen NGV (1974) A cumulant expansion for stochastic linear differential equations. II. Physica 74:239–247

66. Kampen NGV (1985) Elimination of fast variables. Physics Reports 124(2):69–160

67. Kampen NGV (2007) Stochastic processes in physics and chemistry, 3rd edn. North Holland

68. Kampen NGV, Oppenheim I (1986) Brownian motion as a problem of eliminating fast variables. Physica A 138:231–248

69. Kanwal RP (1998) Generalized functions: theory and technique, 2nd edn. Birkhäuser Boston

70. Karimi A, Paul MR (2010) Extensive chaos in the Lorenz-96 model. Chaos 20(4):043,105(1–11)

71. Kato T (1995) Perturbation theory for linear operators, 4th edn. Springer-Verlag

72. Khuri AI (2004) Applications of Dirac's delta function in statistics. Int J Math Educ Sci Technol 35(2):185–195

73. Kraichnan RH (1975) Statistical dynamics of two-dimensional flow. J Fluid Mech 67:155–175

74. Kubo R (1962) Generalized cumulant expansion method. Journal of the physical society of Japan 17(7):1100–1120

75. Kubo R (1963) Stochastic Liouville equations. J Math Phys 4(2):174–183

76. Kullberg A, del Castillo-Negrete D (2012) Transport in the spatially tempered, fractional Fokker-Planck equation. J Phys A: Math Theor 45(25):255,101(1–21)

77. Li G, Wang SW, Rabitz H, Wang S, Jaffé P (2002) Global uncertainty assessments by high dimensional model representations (HDMR). Chemical Engineering Science 57(21):4445–4460

78. Li Z, Bian X, Caswell B, Karniadakis GE (2014) Construction of dissipative particle dynamics models for complex fluids *via* the Mori-Zwanzig formulation. Soft Matter 10:8659–8672

79. Lindenberg K, West BJ, Masoliver J (1989) First passage time problems for non-Markovian processes. In: Moss F, McClintock PVE (eds) Noise in nonlinear dynamical systems (Vol. 1), Cambridge Univ. Press, pp 110–158

80. Lorenz EN (1996) Predictability - A problem partly solved. In: ECMWF seminar on predictability: Volume 1, Reading, pp 1–18

81. Luchtenburg DM, Brunton SL, Rowley CW (2014) Long-time uncertainty propagation using generalized polynomial chaos and flow map composition. J Comp Phys 274:783–802

82. Lundgren TS (1967) Distribution functions in the statistical theory of turbulence. Phys Fluids 10(5):969–975

83. Luo X, Zhu S (2003) Stochastic resonance driven by two different kinds of colored noise in a bistable system. Phys Rev E 67(3/4):021,104(1–13)

84. Ma X, Karniadakis GE (2002) A low-dimensional model for simulating three-dimensional cylinder flow. J Fluid Mech 458:181–190

85. Ma X, Zabaras N (2009) An adaptive hierarchical sparse grid collocation method for the solution of stochastic differential equations. J Comput Phys 228:3084–3113

86. Mattuck RD (1992) A guide to Feynman diagrams in the many-body problem. Dover

87. McCane AJ, Luckock HC, Bray AJ (1990) Path integrals and non-Markov processes. 1. general formalism. Phys Rev A 41(2):644–656

88. McComb WD (1990) The Physics of Fluid Turbulence. Oxford University Press

89. Moler C, Loan CV (2003) Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later. SIAM review 45(1):3–49

90. Monin AS (1967) Equations for turbulent motion. Prikl Mat Mekh 31(6):1057–1068

91. Montgomery D (1976) A BBGKY framework for fluid turbulence. Phys Fluids 19(6):802–810

92. Mori H (1965) Transport, collective motion, and Brownian motion. Prog Theor Phys 33(3):423–455

93. Mori H, Morita T, Mashiyama KT (1980) Contraction of state variables in non-equilibrium open systems. I. Prog Theor Phys 63(6):1865–1883

94. Moss F, McClintock PVE (eds) (1995) Noise in nonlinear dynamical systems. Volume 1: theory of continuous Fokker-Planck systems. Cambridge Univ. Press

95. Mukamel S, Oppenheim I, Ross J (1978) Statistical reduction for strongly driven simple quantum systems. Phys Rev A 17(6):1988–1998

96. Muradoglu M, Jenny P, Pope SB, Caughey DA (1999) A consistent hybrid finite-volume/particle method for the PDF equations of turbulent reactive flows. J Comput Phys 154:342–371

97. Nakajima S (1958) On quantum theory of transport phenomena - steady diffusion. Prog Theor Phys 20(6):948–959

98. Neu P, Speicher R (1993) A self-consistent master equation and a new kind of cumulants. Z Phys B 92:399–407

99. no PE, Warren P (1995) Statistical mechanics of dissipative particle dynamics. Europhys Lett 30(4):191–196

100. Noack BR, Niven RK (2012) A hierarchy of maximum entropy closures for Galerkin systems of incompressible flows. Computers & Mathematics with Applications 65(10):1558–1574

101. Nouy A (2010) Proper generalized decompositions and separated representations for the numerical solution of high dimensional stochastic problems. Arch Comput Methods Appl Mech Eng 17:403–434

102. Nouy A, Maître OPL (2009) Generalized spectral decomposition for stochastic nonlinear problems. J Comput Phys 228:202–235

103. Novak E, Ritter K (1996) High dimensional integration of smooth functions over cubes. Numer Math 75:79–97

104. Novati P (2003) Solving linear initial value problems by Faber polynomials. Numer Linear Algebra Appl 10:247–270

105. Nozaki D, Mar DJ, Grigg P, Collins JJ (1999) Effects of colored noise on stochastic resonance in sensory neurons. Phys Rev Lett 82(11):2402–2405

106. O'Brien EE (1980) The probability density function (pdf) approach to reacting turbulent flows. In: Topics in Applied Physics (Turbulent Reacting Flows), Springer, vol 44, pp 185–218

107. Orszag SA, Bissonnette LR (1967) Dynamical properties of truncated Wiener-Hermite expansions. Phys Fluids 10(12):2603–2613

108. Pereverzev A, Bittner ER (2006) Time-convolutionless master equation for mesoscopic electron-phonon systems. J Chem Phys 125:144,107(1–7)

109. Pesquera L, Rodriguez MA, Santos E (1983) Path integrals for non-Markovian processes. Physics Letters 94(6-7):287–289

110. Pope SB (1981) A Monte Carlo method for the PDF equations of turbulent reactive flow. Combust Sci Technol 25:159–174

111. Pope SB (1994) Lagrangian PDF methods for turbulent flows. Annu Rev Fluid Mech 26:23–63

112. Pope SB (2011) Simple models of turbulent flows. Phys Fluids 23(1):011,301(1–20)

113. Rabitz H, Aliş ÖF, Shorter J, Shim K (1999) Efficient input–output model representations. Computer Physics Communications 117(1-2):11–20

114. Remacle JF, Flaherty JE, Shephard MS (2003) An adaptive discontinuous Galerkin technique with an orthogonal basis applied to compressible flow problems. SIAM Review 45(1):53–72

115. Remacle JF, Flaherty JE, Shephard MS (2003) An adaptive discontinuous Galerkin technique with an orthogonal basis applied to compressible flow problems. SIAM Rev 45(1):53–72

116. Richter M, Knorr A (2010) A time convolution less density matrix approach to the nonlinear optical response of a coupled system-bath complex. Annals of Physics 325:711–747

117. Rjasanow S, Wagner W (2004) Stochastic numerics for the Boltzmann equation. Springer

118. Sapsis TP, Lermusiaux PFJ (2009) Dynamically orthogonal field equations for continuous stochastic dynamical systems. Physica D 238(23-24):2347–2360

119. Snook I (2007) The Langevin and generalised Langevin approach to the dynamics of atomic, polymeric and colloidal systems, 1st edn. Elsevier

120. Stinis P (2006) A comparative study of two stochastic mode reduction methods. Physica D 213:197–213

121. Stinis P (2015) Mori-Zwanzig-reduced models for systems without scale separation. Proc R Soc A 471:20140,446(1–13)

122. Stratonovich RL (1967) Topics in the theory of random noise: Vols. 1 and 2. Gordon and Breach

123. Suzuki M (1985) Decomposition formulas of exponential operators and Lie exponentials with applications to quantum mechanics and statistical physics. J Math Phys 26(4):601–612

124. Suzuki M (1993) General decomposition theory of ordered exponentials. Proc Japan Acad B 69(7):161–166

125. Suzuki M (1994) Convergence of general decompositions of exponential operators. Commun Math Phys 163:491–508

126. Tartakovsky DM, Broyda S (2011) PDF equations for advective-reactive transport in heterogeneous porous media with uncertain properties. Journal of Contaminant Hydrology 120-121:129140

127. Terwiel RH (1974) Projection operator method applied to stochastic linear differential equations. Physica 74:248–265

128. Thalhammer M (2008) High-order exponential operator splitting methods for time-dependent Schrödinger equations. SIAM J Numer Anal 46(4):2022–2038

129. Turkington B (2013) An optimization principle for deriving nonequilibrium statistical models of Hamiltonian dynamics. J Stat Phys 152:569–597

130. Valino L (1998) A field Monte Carlo formulation for calculating the probability density function of a single scalar in a turbulent flow. Flow, Turbul Combust 60(2):157–172

131. Venkatesh TG, Patnaik LM (1993) Effective Fokker-Planck equation: Path-integral formalism. Phys Rev E 48(4):2402–2412

132. Venturi D (2006) On proper orthogonal decomposition of randomly perturbed fields with applications to flow past a cylinder and natural convection over a horizontal plate. J Fluid Mech 559:215–254

133. Venturi D (2011) A fully symmetric nonlinear biorthogonal decomposition theory for random fields. Physica D 240(4-5):415–425

134. Venturi D (2013) Conjugate flow action functionals. J Math Phys 54:113,502(1–19)

135. Venturi D, Karniadakis GE (2012) Differential constraints for the probability density function of stochastic solutions to the wave equation. International Journal for Uncertainty Quantication 2(3):131–150

136. Venturi D, Karniadakis GE (2012) New evolution equations for the joint response-excitation probability density function of stochastic solutions to first-order nonlinear PDEs. J Comput Phys 231:7450–7474

137. Venturi D, Karniadakis GE (2014) Convolutionless Nakajima-Zwanzig equations for stochastic analysis in nonlinear dynamical systems. Proc R Soc A 470(2166):1–20

138. Venturi D, Wan X, Karniadakis GE (2008) Stochastic low-dimensional modelling of a random laminar wake past a circular cylinder. J Fluid Mech 606:339–367

139. Venturi D, Wan X, Karniadakis GE (2010) Stochastic bifurcation analysis of Rayleigh-Bénard convection. J Fluid Mech 650:391–413

140. Venturi D, Choi M, Karniadakis GE (2012) Supercritical quasi-conduction states in stochastic Rayleigh-Bénard convection. Int J Heat and Mass Transfer 55(13-14):3732–3743

141. Venturi D, Sapsis TP, Cho H, Karniadakis GE (2012) A computable evolution equation for the joint response-excitation probability density function of stochastic dynamical systems. Proc R Soc A 468(2139):759–783

142. Venturi D, Tartakovsky DM, Tartakovsky AM, Karniadakis GE (2013) Exact PDF equations and closure approximations for advective-reactive transport. J Comput Phys 243:323–343

143. Villani C (2002) A review of mathematical topics in collisional kinetic theory. In: Friedlander S, Serre D (eds) Handbook of mathematical fluid dynamics, Vol I, North-Holland, Amsterdam, pp 73–258

144. Viswanath D (2004) The fractal property of the lorentz attractor. Physica D 190:115–128

145. Wan X, Karniadakis GE (2005) An adaptive multi-element generalized polynomial chaos method for stochastic differential equations. J Comput Phys 209(2):617–642

146. Wan X, Karniadakis GE (2006) Long-term behavior of polynomial chaos in stochastic flow simulations. Comput Methods Appl Mech Engrg 195:5582–5596

147. Wan X, Karniadakis GE (2006) Multi-element generalized polynomial chaos for arbitrary probability measures. SIAM J Sci Comput 28(3):901–928

148. Wang CJ (2009) Effects of colored noise on stochastic resonance in a tumor cell growth system. Phys Scr 80:065,004 (5pp)

149. Wei J, Norman E (1963) Lie algebraic solutions of linear differential equations. J Math Phys 4(4):575–581

150. Weinberg S (2002) The quantum theory of fields. Volume I. Cambridge University Press

151. Wiebe N, Berry D, Høyer P, Sanders BC (2010) Higher-order decompositions of ordered operator exponentials. J Phys A: Math Theor 43:065,203(1–20)

152. Wilcox RM (1967) Exponential operators and parameter differentiation in quantum physics. J Math Phys 8:399–407

153. Wilczek M, Daitche A, Friedrich R (2011) On the velocity distribution in homogeneous isotropic turbulence: correlations and deviations from Gaussianity. J Fluid Mech 676:191–217

154. Wio HS, Colet P, San Miguel M, Pesquera L, Rodríguez MA (1989) Path-integral formulation for stochastic processes driven by colored noise. Phys Rev A 40(12):7312–7324

155. Xiu D, Karniadakis GE (2002) The Wiener–Askey polynomial chaos for stochastic differential equations. SIAM J Sci Comput 24(2):619–644

156. Xiu D, Karniadakis GE (2003) Modeling uncertainty in flow simulations via generalized polynomial chaos. J Comp Phys 187:137–167

157. Yang Y, Shu CW (2013) Discontinuous Galerkin method for hyperbolic equations involving δ-singularities: negarive-order norma error estimate and applications. Numerische Mathematik 124:753–781

158. Yoshimoto Y, Kinefuchi I, Mima T, Fukushima A, Tokumasu T, Takagi S (2013) Bottom-up construction of interaction models of non-Markovian dissipative particle dynamics. Phys Rev E 88:043,305(1–12)

159. Zwanzig R (1960) Ensemble methods in the theory of irreversibility. J Chem Phys 33(5):1338–1341

160. Zwanzig R (1961) Memory effects in irreversible thermodynamics. Phys Rev 124:983–992