

Uncertainty Quantification for Kinetic Equations



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Abstract Kinetic equations contain uncertainties in their collision kernels or scattering coefficients, initial or boundary data, forcing terms, geometry, etc. Quantifying the uncertainties in kinetic models have important engineering and industrial applications. In this article we survey recent efforts in the study of kinetic equations with random inputs, including their mathematical properties such as regularity and long-time behavior in the random space, construction of efficient stochastic Galerkin methods, and handling of multiple scales by stochastic asymptotic-preserving schemes. The examples used to illustrate the main ideas include the random linear and nonlinear Boltzmann equations, linear transport equation and the Vlasov-Poisson-Fokker-Planck equations.

1 Introduction

Kinetic equations describe the non-equilibrium dynamics of a gas or system comprised of a large number of particles using a probability density function. In multiscale modeling hierarchy, they serve as a basic building block that bridges atomistic and continuum models. On one hand, they are more efficient (requiring fewer degrees of freedom) than molecular dynamics; on the other hand, they provide reliable information at the mesoscopic level when the macroscopic fluid mechanics laws of Navier-Stokes and Fourier become inadequate. The most fundamental (and the very first) kinetic equation is the Boltzmann equation, an integro-differential

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equation describing particle transport and binary collisions [11, 16]. Proposed by Ludwig Boltzmann in 1872, the equation is considered as the basis of the modern kinetic theory. During the past decades, there have been enormous studies on the Boltzmann and related kinetic models, both theoretically and numerically (cf. [13, 20, 74]). This trend is ever-growing as the application of the kinetic theory has already gone beyond traditional fields like rarefied gas dynamics [12], radiative transfer [15], and branched out to microfabrication technology [48, 61], biological and even social sciences [63].

In spite of the vast amount of existing research, the study of kinetic equations has mostly remained deterministic and ignored *uncertainty*. In reality, however, there are many sources of uncertainties that can arise in these equations. They may be due to

- *Incomplete knowledge* of the interaction mechanism between particles. Kinetic equations typically contain an integral operator modeling particle interactions. Inside this integral, there is a term called collision or scattering kernel describing the transition rate during particle collisions. Ideally, the collision kernel should be calculated from first principles using scattering theory [11]. This, if not impossible, is extremely complicated for complex particle systems. Therefore, empirical collision kernels are often used in practice with the aim to reproduce correct viscosity and diffusion coefficients [8, 9, 33, 50]. Specifically, these kernels contain adjustable parameters whose values are determined by matching with available experimental data for various kinds of particles.
- *Imprecise measurement* of the boundary data. A commonly used boundary for kinetic equations is the so-called Maxwell boundary condition [11, 12], which assumes part of the particles are bounced back specularly and part of them are absorbed by the wall and re-emitted according to a special Gaussian distribution. This distribution depends on the (measured) macroscopic properties of the wall such as temperature and bulk velocity.

The uncertainties are of course not limited to the aforementioned examples: they may also come from inaccurate measurement of the initial data, our lack of knowledge of gas-surface interactions, forcing and geometry, etc. Understanding the impact of these uncertainties is critical to the simulations of the complex kinetic systems to validate the kinetic models, and will allow scientists and engineers to obtain more reliable predictions and perform better risk assessment.

Despite tremendous amount of research activities in uncertainty quantification (UQ) in recent decades in many areas of sciences and engineering, the study of uncertainty in kinetic models, albeit important and necessary, has remained mostly untouched territory until very recently. It is the goal of this survey to review recent development of UQ for kinetic equations. Here the uncertainty is introduced through random inputs, and we adopt the generalized polynomial chaos based stochastic Galerkin (gPC-sG) approximation, which has been successfully applied to many physical and engineering problems, see for instance, the overviews in [27, 55, 66, 77]. Due to the high-dimensionality and intrinsic physical properties of kinetic equations, the construction of stochastic methods represents a great

challenge. We will use some prototype equations including the classical Boltzmann equation, linear Boltzmann equations, and Vlasov-Poisson-Fokker-Planck system to illustrate the main strategy.

It is well-known that the gPC-sG approach is intrusive, requiring more coding efforts compared with non-intrusive methods such as the stochastic collocation [32, 78]. The reason of our choice is twofold: (1) Due to its Galerkin formulation, mathematical analysis of these methods can be conducted more conveniently. Indeed many of the analytical methods well-established in kinetic theory can be conveniently adopted or extended to study the stochastic Galerkin system of the random kinetic equations; (2) Kinetic equations often contain small parameters such as the mean free path/time which asymptotically lead to hyperbolic/diffusion equations. We are interested in developing the stochastic analogue of the asymptotic-preserving (AP) scheme, a scheme designed to capture the asymptotic limit at the discrete level. The stochastic Galerkin method yields systems of deterministic equations that *resemble the deterministic kinetic equations*, although in vector forms. Thus it allows one to easily use the deterministic AP framework for the random problems, allowing minimum “intrusivity” to the legacy deterministic codes. The stochastic Galerkin method can ensure the desired convergence in the weak sense. The resulting stochastic Asymptotic-Preserving (sAP) [46] sG methods will allow all numerical parameters, such as mesh size, time-step and the number of gPC modes chosen *independently* of the (possibly small) mean free path/time.

On the other hand, the study of regularity, coercivity and hypocoercivity on the random kinetic equations, which will be reviewed in this article as well, provides theoretical foundation for not only the stochastic Galerkin methods, but also the stochastic collocation methods.

The rest of this paper is organized as follows. In the next section, we give a brief review of some kinetic equations with random inputs and their basic properties. Section 3 discusses the theoretical issues such as coercivity, hypocoercivity, regularity, and long-time behavior for random kinetic equations. We then introduce in Sect. 4 the gPC-sG method. Special emphasis is given to the unique issues arising in kinetic equations such as property of the collision operator under gPC-sG approximation and efficient treatment of the nonlinear collision integral. Spectral accuracy of the gPC-sG method is also established. In Sect. 5, we consider the kinetic equations in diffusive scalings and construct the stochastic AP scheme following its deterministic counterpart. We conclude in Sect. 6 and list a few open problems in this field.

2 Preliminaries on Kinetic Equations with Random Inputs

In this section, we review some kinetic equations and their basic properties that will be used in this article. Due to the large variety of kinetic models, it is impossible to give a thorough description of all of them. Therefore, we will concentrate on several prototype models: the linear neutron transport equation, the semiconductor Boltzmann equation, the Vlasov-Poisson-Fokker-Planck equation,

and the classical nonlinear Boltzmann equation. Other related kinetic models will be briefly mentioned at the end of the section.

As mentioned in Sect. 1, for real-world problems, the collision/scattering kernel, initial/boundary data, source, or other physical parameters in the kinetic equations may contain uncertainties that propagate into the solution and affect its property substantially. To characterize these random inputs, we assume certain quantities depend on a random vector $\mathbf{z} \in \mathbb{R}^n$ in a properly defined probability space $(\Sigma, \mathcal{A}, \mathbb{P})$, whose event space is Σ and is equipped with σ -algebra \mathcal{A} and probability measure \mathbb{P} . We also assume the components of \mathbf{z} are mutually independent random variables with known probability $\omega(\mathbf{z}) : I_{\mathbf{z}} \rightarrow \mathbb{R}^+$, obtained already through some dimension reduction technique, e.g., Karhunen-Loève (KL) expansion [60], and do not pursue further the issue of random input parameterization. We treat \mathbf{z} as a parameter and the properties given in this section hold for every given \mathbf{z} .

2.1 The Linear Transport Equation with Isotropic Scattering

We first introduce the linear transport equation in one dimensional slab geometry:

$$\varepsilon \partial_t f + v \partial_x f = \frac{\sigma}{\varepsilon} \mathcal{L}f - \varepsilon \sigma^a f + \varepsilon S, \quad t > 0, x \in [0, 1], v \in [-1, 1], \mathbf{z} \in I_{\mathbf{z}}, \quad (1)$$

$$\mathcal{L}f(t, x, v, \mathbf{z}) = \frac{1}{2} \int_{-1}^1 f(t, x, v', \mathbf{z}) dv' - f(t, x, v, \mathbf{z}), \quad (2)$$

with the initial condition

$$f(0, x, v, \mathbf{z}) = f^0(x, v, \mathbf{z}). \quad (3)$$

This equation arises in neutron transport, radiative transfer, etc. and describes particles (for example neutrons) transport in a background media (for example nuclei). $f(t, x, v, \mathbf{z})$ is the density distribution of particles at time t , position x , and $v = \Omega \cdot e_x = \cos \theta$ where θ is the angle between the moving direction and x -axis. $\sigma(x, \mathbf{z})$, $\sigma^a(x, \mathbf{z})$ are total and absorption cross-sections respectively. $S(x, \mathbf{z})$ is the source term. For $\sigma(x, \mathbf{z})$, we assume

$$\sigma(x, \mathbf{z}) \geq \sigma_{\min} > 0. \quad (4)$$

ε is the dimensionless Knudsen number, the ratio between particle mean free path and the characteristic length (such as the length of the domain). The equation is scaled in long time with strong scattering.

We are interested in problems that contain *uncertainties* in the collision cross-section, source, initial or boundary data. Thus in our problem f , σ , σ^a and S all depend on \mathbf{z} .

Denote

$$[\phi] = \frac{1}{2} \int_{-1}^1 \phi(v) dv \quad (5)$$

as the average of a velocity dependent function ϕ .

Define in the Hilbert space $L^2([-1, 1]; \phi^{-1} dv)$ the inner product and norm

$$\langle f, g \rangle_\phi = \int_{-1}^1 f(v)g(v)\phi^{-1} dv, \quad \|f\|_\phi^2 = \langle f, f \rangle_\phi. \quad (6)$$

The linear operator \mathcal{L} satisfies the following properties [6]:

- $[\mathcal{L}f] = 0$, for every $f \in L^2([-1, 1])$;
- The null space of f is $\mathcal{N}(\mathcal{L}) = \text{Span} \{ \phi \mid \phi = [\phi] \}$;
- The range of f is $\mathcal{R}(\mathcal{L}) = \mathcal{N}(\mathcal{L})^\perp = \{ f \mid [f] = 0 \}$;
- *Coercivity*: \mathcal{L} is non-positive self-adjoint in $L^2([-1, 1]; \phi^{-1} dv)$, i.e., there is a positive constant s_m such that

$$\langle f, \mathcal{L}f \rangle_\phi \leq -2s_m \|f\|_\phi^2, \quad \forall f \in \mathcal{N}(\mathcal{L})^\perp; \quad (7)$$

- \mathcal{L} admits a pseudo-inverse, denoted by \mathcal{L}^{-1} , from $\mathcal{R}(\mathcal{L})$ to $\mathcal{R}(\mathcal{L})$.

Let $\rho = [f]$. For each fixed \mathbf{z} , the classical diffusion limit theory of linear transport equation [6, 7, 52] gives that, as $\varepsilon \rightarrow 0$, ρ solves the following diffusion equation:

$$\partial_t \rho = \partial_x (\kappa(x, \mathbf{z}) \partial_x \rho) - \sigma^a(x, \mathbf{z}) \rho + S(x, \mathbf{z}), \quad (8)$$

where the diffusion coefficient

$$\kappa(x, \mathbf{z}) = \frac{1}{3} \sigma(x, \mathbf{z})^{-1}. \quad (9)$$

When \mathbf{z} is random, (8) is a random diffusion equation.

2.2 The Semiconductor Boltzmann Equation

The semiconductor Boltzmann equation describes the electron transport in a semiconductor device [61]:

$$\varepsilon \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \nabla_{\mathbf{x}} \phi \cdot \nabla_{\mathbf{v}} f = \frac{1}{\varepsilon} \mathcal{Q}^s(f), \quad t > 0, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad \mathbf{v} \in \mathbb{R}^d, \quad \mathbf{z} \in I_{\mathbf{z}}, \quad (10)$$

where $f(t, \mathbf{x}, \mathbf{v}, \mathbf{z})$ is again the particle distribution function, $\phi(t, \mathbf{x}, \mathbf{z})$ is the electric potential given a priori or produced self-consistently by f through the Poisson equation:

$$\Delta_{\mathbf{x}}\phi = \rho - h,$$

where $\rho(t, \mathbf{x}, \mathbf{z}) = \int f \, d\mathbf{v}$, and $h(\mathbf{x}, \mathbf{z})$ is the doping profile (some physical parameters such as the material permittivity are omitted for brevity). The collision operator $\mathcal{Q}^s(f)$ is a linear approximation of the electron-phonon interaction:

$$\mathcal{Q}^s(f)(\mathbf{v}, \mathbf{z}) = \int_{\mathbb{R}^d} [s(\mathbf{v}_*, \mathbf{v}, \mathbf{z})f(\mathbf{v}_*, \mathbf{z}) - s(\mathbf{v}, \mathbf{v}_*, \mathbf{z})f(\mathbf{v}, \mathbf{z})] \, d\mathbf{v}_*, \quad (11)$$

where $s(\mathbf{v}, \mathbf{v}_*, \mathbf{z})$ describes the transition rate from \mathbf{v} to \mathbf{v}_* and may take various forms depending on the approximation. Here we assume

$$s(\mathbf{v}, \mathbf{v}_*, \mathbf{z}) = \sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z})M^s(\mathbf{v}_*),$$

with M^s being the normalized Maxwellian:

$$M^s(\mathbf{v}) = \frac{1}{\pi^{d/2}} e^{-|\mathbf{v}|^2};$$

the scattering kernel σ being rotationally invariant, symmetric and bounded:

$$\sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z}) = \sigma(|\mathbf{v}|, |\mathbf{v}_*|, \mathbf{z}), \quad 0 < \sigma_{\min} \leq \sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z}) = \sigma(\mathbf{v}_*, \mathbf{v}, \mathbf{z}) \leq \sigma_{\max}.$$

Define the collision frequency

$$\lambda(\mathbf{v}, \mathbf{z}) = \int_{\mathbb{R}^d} \sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z})M^s(\mathbf{v}_*) \, d\mathbf{v}_*, \quad (12)$$

then it is easy to see $\sigma_0 \leq \lambda(\mathbf{v}, \mathbf{z}) \leq \sigma_1$. Therefore, (11) can be written as

$$\begin{aligned} \mathcal{Q}^s(f)(\mathbf{v}, \mathbf{z}) &= \int_{\mathbb{R}^d} \sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z}) [M^s(\mathbf{v})f(\mathbf{v}_*, \mathbf{z}) - M^s(\mathbf{v}_*)f(\mathbf{v}, \mathbf{z})] \, d\mathbf{v}_* \\ &= M^s(\mathbf{v}) \int_{\mathbb{R}^d} \sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z})f(\mathbf{v}_*, \mathbf{z}) \, d\mathbf{v}_* - \lambda(\mathbf{v}, \mathbf{z})f(\mathbf{v}, \mathbf{z}). \end{aligned} \quad (13)$$

It can be shown that the collision operator (13) satisfies

$$\begin{aligned} &\int_{\mathbb{R}^d} \mathcal{Q}^s(f)(\mathbf{v}, \mathbf{z})f(\mathbf{v}, \mathbf{z})/M^s(\mathbf{v}) \, d\mathbf{v} \\ &= -\frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z})M^s(\mathbf{v})M^s(\mathbf{v}_*) \left(\frac{f(\mathbf{v})}{M^s(\mathbf{v})} - \frac{f(\mathbf{v}_*)}{M^s(\mathbf{v}_*)} \right)^2 \, d\mathbf{v}_*d\mathbf{v} \leq 0. \end{aligned} \quad (14)$$

Furthermore, the followings are equivalent

$$\int_{\mathbb{R}^d} \mathcal{Q}^s(f) \frac{f}{M} d\mathbf{v} = 0 \iff \mathcal{Q}^s(f) = 0 \iff f = \rho(t, \mathbf{x}, \mathbf{z}) M^s(\mathbf{v}). \quad (15)$$

Then, as $\varepsilon \rightarrow 0$, (10) leads to the following *drift-diffusion* limit [67]:

$$\partial_t \rho = \nabla_{\mathbf{x}} \cdot (D (\nabla_{\mathbf{x}} \rho + 2\rho \mathbf{E})), \quad (16)$$

where $\mathbf{E} = -\nabla_{\mathbf{x}} \phi$ is the electric field, D is the diffusion coefficient matrix defined by

$$D = \int_{\mathbb{R}^d} \frac{\mathbf{v} \otimes \mathbf{v} M^s(\mathbf{v})}{\lambda(\mathbf{v}, \mathbf{z})} d\mathbf{v}.$$

2.3 The Vlasov-Poisson-Fokker-Planck System

The Vlasov-Poisson-Fokker-Planck (VPFP) system arises in the kinetic modeling of the Brownian motion of a large system of particles in a surrounding bath [14]. One application of such system is the electrostatic plasma, in which one considers the interactions between the electrons and a surrounding bath via the Coulomb force. In the dimensionless VPFP system with uncertainty, the time evolution of particle density distribution function $f(t, \mathbf{x}, \mathbf{v}, \mathbf{z})$ under the action of an electrical potential $\phi(t, \mathbf{x}, \mathbf{z})$ satisfies

$$\begin{cases} \partial_t f + \frac{1}{\delta} \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \frac{1}{\varepsilon} \nabla_{\mathbf{x}} \phi \cdot \nabla_{\mathbf{v}} f = \frac{1}{\delta \varepsilon} \mathcal{F} f, \\ -\Delta_{\mathbf{x}} \phi = \rho - 1, \quad t > 0, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad \mathbf{v} \in \mathbb{R}^d, \quad \mathbf{z} \in I_{\mathbf{z}}, \end{cases} \quad (17)$$

with initial condition

$$f(0, \mathbf{x}, \mathbf{v}, \mathbf{z}) = f^0(\mathbf{x}, \mathbf{v}, \mathbf{z}). \quad (18)$$

Here, \mathcal{F} is a collision operator describing the Brownian motion of the particles, which reads,

$$\mathcal{F} f = \nabla_{\mathbf{v}} \cdot \left(M^v \nabla_{\mathbf{v}} \left(\frac{f}{M^v} \right) \right), \quad (19)$$

where M^v is the *global equilibrium* or *global Maxwellian*,

$$M^v = \frac{1}{(2\pi)^{\frac{d}{2}}} e^{-\frac{|\mathbf{v}|^2}{2}}. \quad (20)$$

δ is the reciprocal of the scaled thermal velocity, ε represents the scaled thermal mean free path. There are two different regimes for this system. One is the *high field regime*, where $\delta = 1$. As $\varepsilon \rightarrow 0$, f goes to the local Maxwellian $M_l^v = \frac{1}{(2\pi)^{\frac{d}{2}}} e^{-\frac{|\mathbf{v} - \nabla_{\mathbf{x}}\phi|^2}{2}}$, and the VPFP system converges to a hyperbolic limit [2, 31, 65]:

$$\begin{cases} \partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \nabla_{\mathbf{x}} \phi) = 0, \\ -\Delta_{\mathbf{x}} \phi = \rho - 1. \end{cases} \quad (21)$$

Another regime is the *parabolic regime*, where $\delta = \varepsilon$. When $\varepsilon \rightarrow 0$, f goes to the global Maxwellian M^v , and the VPFP system converges to a parabolic limit [68]:

$$\begin{cases} \partial_t \rho - \nabla_{\mathbf{x}} \cdot (\nabla_{\mathbf{x}} \rho - \rho \nabla_{\mathbf{x}} \phi) = 0, \\ -\Delta_{\mathbf{x}} \phi = \rho - 1. \end{cases} \quad (22)$$

2.4 The Classical Nonlinear Boltzmann Equation

We finally introduce the classical Boltzmann equation that describes the time evolution of a rarefied gas [11]:

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \mathcal{Q}^b(f, f), \quad t > 0, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad \mathbf{v} \in \mathbb{R}^d, \quad \mathbf{z} \in I_{\mathbf{z}}, \quad (23)$$

where $\mathcal{Q}^b(f, f)$ is the bilinear collision operator modeling the binary interaction among particles:

$$\mathcal{Q}^b(f, f)(\mathbf{v}, \mathbf{z}) = \int_{\mathbb{R}^d} \int_{S^{d-1}} B(\mathbf{v}, \mathbf{v}_*, \eta, \mathbf{z}) [f(\mathbf{v}', \mathbf{z})f(\mathbf{v}'_*, \mathbf{z}) - f(\mathbf{v}, \mathbf{z})f(\mathbf{v}_*, \mathbf{z})] d\eta d\mathbf{v}_*. \quad (24)$$

Here $(\mathbf{v}, \mathbf{v}_*)$ and $(\mathbf{v}', \mathbf{v}'_*)$ are the velocity pairs before and after a collision, during which the momentum and energy are conserved; hence $(\mathbf{v}', \mathbf{v}'_*)$ can be represented in terms of $(\mathbf{v}, \mathbf{v}_*)$ as

$$\begin{cases} \mathbf{v}' = \frac{\mathbf{v} + \mathbf{v}_*}{2} + \frac{|\mathbf{v} - \mathbf{v}_*|}{2} \eta, \\ \mathbf{v}'_* = \frac{\mathbf{v} + \mathbf{v}_*}{2} - \frac{|\mathbf{v} - \mathbf{v}_*|}{2} \eta, \end{cases}$$

with the parameter η varying on the unit sphere S^{d-1} . The collision kernel $B(\mathbf{v}, \mathbf{v}_*, \eta, \mathbf{z})$ is a non-negative function depending on $|\mathbf{v} - \mathbf{v}_*|$ and cosine of the

deviation angle θ :

$$B(\mathbf{v}, \mathbf{v}_*, \eta, \mathbf{z}) = B(|\mathbf{v} - \mathbf{v}_*|, \cos \theta, \mathbf{z}), \quad \cos \theta = \frac{\eta \cdot (\mathbf{v} - \mathbf{v}_*)}{|\mathbf{v} - \mathbf{v}_*|}.$$

The specific form of B is determined from the intermolecular potential via the scattering theory. For numerical purpose, a commonly used model is the variable hard-sphere (VHS) model introduced by Bird [9]:

$$B(|\mathbf{v} - \mathbf{v}_*|, \cos \theta, \mathbf{z}) = b_\lambda(\mathbf{z})|\mathbf{v} - \mathbf{v}_*|^\lambda, \quad -d < \lambda \leq 1, \quad (25)$$

where $\lambda > 0$ corresponds to the hard potentials, and $\lambda < 0$ to the soft potentials.

The collision operator (24) conserves mass, momentum, and energy:

$$\int_{\mathbb{R}^d} \mathcal{Q}^b(f, f) \, d\mathbf{v} = \int_{\mathbb{R}^d} \mathcal{Q}^b(f, f) \mathbf{v} \, d\mathbf{v} = \int_{\mathbb{R}^d} \mathcal{Q}^b(f, f) |\mathbf{v}|^2 \, d\mathbf{v} = 0. \quad (26)$$

It satisfies the celebrated Boltzmann's H -theorem:

$$-\int_{\mathbb{R}^d} \mathcal{Q}^b(f, f) \ln f \, d\mathbf{v} \geq 0,$$

which implies that the entropy is always non-decreasing. Furthermore, the following statements are equivalent

$$\int_{\mathbb{R}^d} \mathcal{Q}^b(f, f) \ln f \, d\mathbf{v} = 0 \iff \mathcal{Q}^b(f, f) = 0 \iff f = \mathcal{M}^b(\mathbf{v})_{(\rho(t, \mathbf{x}, \mathbf{z}), \mathbf{u}(t, \mathbf{x}, \mathbf{z}), T(t, \mathbf{x}, \mathbf{z}))},$$

where \mathcal{M}^b is the local equilibrium/Maxwellian defined by

$$\mathcal{M}^b = \frac{\rho}{(2\pi T)^{d/2}} e^{-\frac{(\mathbf{v}-\mathbf{u})^2}{2T}},$$

with ρ , \mathbf{u} , T being, respectively, the density, bulk velocity, and temperature:

$$\rho = \int_{\mathbb{R}^d} f \, d\mathbf{v}, \quad \mathbf{u} = \frac{1}{\rho} \int_{\mathbb{R}^d} f \mathbf{v} \, d\mathbf{v}, \quad T = \frac{1}{d\rho} \int_{\mathbb{R}^d} f |\mathbf{v} - \mathbf{u}|^2 \, d\mathbf{v}. \quad (27)$$

A widely used boundary condition for Boltzmann-like kinetic equations is the Maxwell boundary condition which is a linear combination of specular reflection and diffusion (particles are absorbed by the wall and then re-emitted according to a Maxwellian distribution of the wall). Specifically, for any boundary point $\mathbf{x} \in \partial\Omega$, let $n(\mathbf{x})$ be the unit normal vector to the boundary, pointed to the domain, then the in-flow boundary condition is given by

$$f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) = g(t, \mathbf{x}, \mathbf{v}, \mathbf{z}), \quad (\mathbf{v} - \mathbf{u}_w) \cdot n > 0,$$

with

$$\begin{aligned}
 g(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) = & (1 - \alpha)f(t, \mathbf{x}, \mathbf{v} - 2[(\mathbf{v} - \mathbf{u}_w) \cdot \mathbf{n}]\mathbf{n}, \mathbf{z}) \\
 & + \frac{\alpha}{(2\pi)^{\frac{d-1}{2}} T_w^{\frac{d+1}{2}}} e^{-\frac{|\mathbf{v} - \mathbf{u}_w|^2}{2T_w}} \int_{(\mathbf{v} - \mathbf{u}_w) \cdot \mathbf{n} < 0} f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) |(\mathbf{v} - \mathbf{u}_w) \cdot \mathbf{n}| \, d\mathbf{v},
 \end{aligned} \tag{28}$$

where $\mathbf{u}_w = \mathbf{u}_w(t, \mathbf{x}, \mathbf{z})$, $T_w = T_w(t, \mathbf{x}, \mathbf{z})$ are the velocity and temperature of the wall (boundary). The constant α ($0 \leq \alpha \leq 1$), which may depend on \mathbf{z} as well, is the accommodation coefficient with $\alpha = 1$ corresponding to the purely diffusive boundary, and $\alpha = 0$ the purely specular reflective boundary.

2.5 Other Related Kinetic Models: A Glance

In addition to the above introduced equations, we mention a few related kinetic models. Interested readers may consult the survey papers [11, 20, 74] for details. First of all, the collision operator does not have to be the aforementioned forms: when the deviation angle θ is small, the Boltzmann collision integral (24) diverges and one has to consider its grazing collision limit—the Fokker-Planck-Landau operator [51], which is a diffusive operator relevant in the study of Coulomb interactions. When the quantum effect is non-negligible (particles behave as Bosons or Fermions), (11) or (24) needs to be modified to include an extra factor like $(1 \pm f)$, resulting in the so-called quantum or degenerate collision operators [19, 73]. Other generalizations such as the multi-species model [71] (system consists of more than one type of particles), inelastic model [75] (during collisions only the mass and momentum are conserved whereas the energy is dissipative, for example, in granular materials) are also possible. Secondly, the forcing term on the left hand side is not necessary as that shown in (10): generally one can couple the kinetic equation with the Maxwell equation where both electric and magnetic effects are present [72].

3 Coercivity, Hypocoercivity, Regularity and Long Time Behavior

Coercivity, or more generally hypocoercivity, describing the dissipative nature of the kinetic collision operators, plays important roles in the study of the solution of kinetic equations toward the local or global Maxwellian [74, 76]. For uncertain problems, one can extend such behavior to the random space, thus gives rise to regularity or long-time estimates in the random space of the solution, allowing one to quantify the long-time impact of the uncertainties for some statistical quantities

of interest. In this section, we will review some of recent results in this direction, in particular, how such analysis can be used to understand the regularity and propagation of uncertainty for random kinetic equations.

In this section we will restrict our discussion to the one-dimensional random variable z with finite support I_z (e.g., uniform and beta distributions). Generalization to multi-dimensional random variables with finite support can be carried out in a similar fashion.

3.1 The Linear Transport Equation

To study the regularity and long-time behavior in the random space of the linear transport equation (1)–(3), we first recall the Hilbert space of the random variable

$$H(I_z; \omega \, dz) = \left\{ f \mid I_z \rightarrow \mathbb{R}^+, \int_{I_z} f^2(z) \omega(z) \, dz < +\infty \right\}, \quad (29)$$

equipped with the inner product and norm defined as

$$\langle f, g \rangle_\omega = \int_{I_z} fg \, \omega(z) \, dz, \quad \|f\|_\omega^2 = \langle f, f \rangle_\omega. \quad (30)$$

We also define the k th order differential operator with respect to z as

$$D^k f(t, x, v, z) := \partial_z^k f(t, x, v, z), \quad (31)$$

and the Sobolev norm in H as

$$\|f(t, x, v, \cdot)\|_{H^k}^2 := \sum_{\alpha \leq k} \|D^\alpha f(t, x, v, \cdot)\|_\omega^2. \quad (32)$$

Finally, we introduce norms in space and velocity as follows,

$$\|f(t, \cdot, \cdot, \cdot)\|_{L^2}^2 := \int_Q \|f(t, x, v, \cdot)\|_\omega^2 \, dx \, dv, \quad t \geq 0, \quad (33)$$

$$\|f(t, \cdot, \cdot, \cdot)\|_{L^2}^2 := \int_Q \|f(t, x, v, \cdot)\|_{H^k}^2 \, dx \, dv, \quad t \geq 0, \quad (34)$$

where $Q = [0, 1] \times [-1, 1]$ denotes the domain in the phase space. For simplicity, we will suppress the dependence of t and just use $\|f\|_{L^2}$, $\|f\|_{L^2}^k$ in the following proof.

An important property of \mathcal{L} is its coercivity, given in (7), based on which the following results were established in [47].

Theorem 1 (Uniform Regularity) *If for some integer $m \geq 0$,*

$$\|D^k \sigma(z)\|_{L^\infty} \leq C_\sigma, \quad \|D^k f_0\|_\Gamma \leq C_0, \quad k = 0, \dots, m, \quad (35)$$

then the solution f to the linear transport equation (1)–(3), with $\sigma^a = S = 0$ and periodic boundary condition in x , satisfies,

$$\|D^k f\|_\Gamma \leq C, \quad k = 0, \dots, m, \quad \forall t > 0, \quad (36)$$

where C_σ , C_0 and C are constants independent of ε .

The above theorem shows that, under some smoothness assumption on σ , the regularity of the initial data is preserved in time and the Sobolev norm of the solution is bounded uniformly in ε .

Theorem 2 (ε^2 -Estimate on $[f] - f$) *With all the assumptions in Theorem 1 and furthermore, $\sigma \in W^{k,\infty} = \{\sigma \in L^\infty([0, 1] \times I_z) \mid D^j \sigma \in L^\infty([0, 1] \times I_z) \text{ for all } j \leq k\}$. For a given time $T > 0$, the following regularity result of $[f] - f$ holds:*

$$\|D^k([f] - f)\|_\Gamma^2 \leq e^{-\sigma_{\min} t / 2\varepsilon^2} \|D^k([f_0] - f_0)\|_\Gamma^2 + C' \varepsilon^2 \quad (37)$$

for any $t \in (0, T]$ and $0 \leq k \leq m$, where C' and C are constants independent of ε .

The first term on the right hand side of (37) is the behavior of the initial layer, which is damped exponentially in t/ε . After the initial layer, the high order derivatives in z of the difference between f and its local equilibrium $[f]$ is of $O(\varepsilon)$.

3.2 The Semiconductor Boltzmann Equation

The results in the previous subsection can be extended to the (linear) semiconductor Boltzmann equation by assuming $\phi = 0$ in (10).

Introduce the Hilbert space of the velocity variable $L_M^2 := L^2\left(\mathbb{R}^d; \frac{dv}{M^s(v)}\right)$, with the corresponding inner product $\langle \cdot, \cdot \rangle_{L_M^2}$ and norm $\|\cdot\|_{L_M^2}$. First, the collision operator \mathcal{Q}^s has the following *coercivity* property for any $f \in L_M^2$ [69],

$$\langle \mathcal{Q}^s(f), f \rangle_{L_M^2} \leq -\sigma_{\min} \|f - \rho M^s\|_{L_M^2}^2, \quad (38)$$

Introduce the following norms

$$\|f(t, \cdot, \cdot, \cdot)\|_\Gamma^2 := \int_\Omega \int_{\mathbb{R}^d} \frac{\|f\|_\omega^2}{M(v)} dv dx,$$

$$\|f(t, \cdot, \cdot, \cdot)\|_{\Gamma^k}^2 := \int_\Omega \int_{\mathbb{R}^d} \frac{\|f\|_{H^k}^2}{M(v)} dv dx.$$

We assume a periodic boundary condition in space. The following results were proved in [59].

Theorem 3 (Uniform Regularity) *Assume for some integer $m \geq 0$,*

$$\|D^k \sigma\|_{L^\infty(v,z)} \leq C_\sigma, \quad \|D^k f_0\|_{\Gamma} \leq C_0, \quad k = 0, \dots, m,$$

then the solution f to (10) satisfies

$$\|D^k f\|_{\Gamma} \leq C, \quad k = 0, \dots, m, \quad \forall t > 0,$$

where C_σ , C_0 and C are constants independent of ε .

Theorem 4 (Estimate on $f - \rho M^s$) *With all the assumptions in Theorem 3, and in addition,*

$$\begin{aligned} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (D^k \sigma) v^2 M^s(v) M^s(w) dw dv &\leq C, \\ \left| \int_{\mathbb{R}^d} (D^k \sigma) M^s(w) dw \right| &\leq C, \quad \|D^k (v \cdot \nabla_x f_0)\|_{\Gamma} \leq C, \end{aligned}$$

for $k = 1, \dots, m$, then

$$\|D^k (f - \rho M^s)\|_{\Gamma}^2 \leq e^{-\sigma_{\min} t / 2\varepsilon^2} \|D^k (f_0 - \rho_0 M_0^s)\|_{\Gamma}^2 + C' \varepsilon^2 \leq C \varepsilon^2, \quad (39)$$

for any $t \in (0, T]$ and $0 \leq k \leq m$, where C' and C are constants independent of ε .

Differing from the isotropic scattering, for the anisotropic collision kernel, to obtain the decay rate of $f - \rho M^s$, an exponential decay estimate on $v \cdot \nabla_x f$ is needed [59].

3.3 General Linear Kinetic Equations

While the previous analysis gave decay estimates on the deviation between f and its *local equilibrium*, which can be difficult for more general kinetic equations, the use of *hypocoercivity* to estimate the deviation of f from the *global equilibrium* which is independent of t and x , helps one to deal with more general and even nonlinear equations. For general linear transport equation with *one* conserved quantity:

$$\partial_t f + \frac{1}{\varepsilon} \mathbf{v} \cdot \nabla_x f + \frac{1}{\varepsilon} \nabla_x \phi \cdot \nabla_v f = \frac{1}{\delta \varepsilon} \mathcal{Q}^l(f), \quad (40)$$

where the collision \mathcal{Q}^l includes

- BGK operator $\mathcal{Q}^l = \sigma(x, z)(\Pi f - f)$, where Π is a projection operator onto the local equilibrium;

- Anisotropic scattering operator $\mathcal{Q}^l = \int [\sigma(v \rightarrow v^*, z)f(v^*) - \sigma(v^* \rightarrow v, z)f(v)] dv^*$, $\sigma > 0$.

Two regimes will be considered: the high-field regime ($\delta = 1$) and the parabolic regime ($\delta = \varepsilon$).

In [57] the following regularity result was established:

Theorem 5 *Let f be the solution to the kinetic equation (40), and assume the initial data has sufficient regularity with respect to z : $\|\partial_z^l f_0\| \leq H^l$, then:*

- (1) $\|\partial_z^l f\| \leq Cl! \min\{e^{-\lambda_z t} C(t)^l, e^{(C-\lambda_z)t} 2^{l-1} (1+H)^{l+1}\}$, where C is a constant, $C(t)$ is an algebraic function of t , and $\lambda_z > 0$ is uniformly bounded below from zero;
- (2) f is analytic with uniform convergence radius $\frac{1}{2(1+H)}$;
- (3) Both the exponential convergence in time and convergence radius are uniform with respect to ε .

The proof of the results is based on the hypocoercivity property for deterministic equation [21], which gives the exponential decay in time, and a careful analysis of ε -independent decay rate.

3.4 The Vlasov-Poisson-Fokker-Planck System

We now discuss the (*nonlinear*) VPFP system (17)–(18). For simplicity, we only consider $\mathbf{x} = x \in (0, l)$ and $\mathbf{v} = v \in \mathbb{R}$ in one dimension. Define the L^2 space in the measure of

$$d\mu = d\mu(x, v, z) = \omega(z) dx dv dz. \quad (41)$$

With this measure, one has the corresponding Hilbert space with the following inner product and norms:

$$\langle f, g \rangle = \int_{\Omega} \int_{\mathbb{R}} \int_{I_z} fg d\mu(x, v, z), \quad \text{or,} \quad \langle \rho, j \rangle = \int_{\Omega} \int_{I_z} \rho j d\mu(x, z), \quad (42)$$

with norm

$$\|f\|^2 = \langle f, f \rangle.$$

In order to get the convergence rate of the solution to the global equilibrium, define,

$$h = \frac{f - M^v}{\sqrt{M^v}}, \quad \sigma = \int_{\mathbb{R}} h \sqrt{M} dv, \quad u = \int_{\mathbb{R}} h v \sqrt{M} dv, \quad (43)$$

where h is the (microscopic) *fluctuation* around the equilibrium, σ is the (macroscopic) density fluctuation, and u is the (macroscopic) velocity fluctuation. Then the microscopic quantity h satisfies,

$$\varepsilon \delta \partial_t h + \beta v \partial_x h - \delta \partial_x \phi \partial_v h + \delta \frac{v}{2} \partial_x \phi h + \delta v \sqrt{M} \partial_x \phi = \mathcal{L}^F h, \quad (44)$$

$$\partial_x^2 \phi = -\sigma, \quad (45)$$

while the macroscopic quantities σ and u satisfy

$$\delta \partial_t \sigma + \partial_x u = 0, \quad (46)$$

$$\varepsilon \delta \partial_t u + \varepsilon \partial_x \sigma + \varepsilon \int v^2 \sqrt{M} (1 - \Pi) \partial_x h dv + \delta \partial_x \phi \sigma + u + \delta \partial_x \phi = 0, \quad (47)$$

where \mathcal{L}^F is the so-called linearized Fokker-Planck operator,

$$\mathcal{L}^F h = \frac{1}{\sqrt{M^v}} \mathcal{F} \left(M^v + \sqrt{M^v} h \right) = \frac{1}{\sqrt{M^v}} \partial_v \left(M^v \partial_v \left(\frac{h}{\sqrt{M^v}} \right) \right). \quad (48)$$

Introduce projections onto $\sqrt{M^v}$ and $v \sqrt{M^v}$,

$$\Pi_1 h = \sigma \sqrt{M^v}, \quad \Pi_2 h = v u \sqrt{M^v}, \quad \Pi h = \Pi_1 h + \Pi_2 h. \quad (49)$$

Furthermore, we also define the following norms and energies,

- Norms:

- $\|h\|_{L^2(v)}^2 = \int_{\mathbb{R}} h^2 dv,$
- $\|f\|_{H^m}^2 = \sum_{l=0}^m \|\partial_x^l f\|^2, \quad \|f\|_{H^1(x,z)}^2 = \|f\|^2 + \|\partial_x f\|^2 + \|\partial_z f\|^2,$
- $\|h\|_v^2 = \int_{(0,l) \times \mathbb{R} \times I_z} (\partial_v h)^2 + (1 + |v|^2) h^2 d\mu(x, v, z), \quad \|h\|_{H_v^m}^2 = \sum_{l=0}^m \|\partial_x^l h\|_v^2;$

- Energy terms:

- $E_h^m = \|h\|_{H^m}^2 + \|\partial_x h\|_{H^{m-1}}^2, \quad E_\phi^m = \|\partial_x \phi\|_{H^m}^2 + \|\partial_x^2 \phi\|_{H^{m-1}}^2;$

- Dissipation terms:

- $D_h^m = \|(1 - \Pi)h\|_{H^m}^2 + \|(1 - \Pi)\partial_x h\|_{H^{m-1}}^2, \quad D_\phi^m v = E_\phi^m v,$
- $D_u^m = \|u\|_{H^m}^2 + \|\partial_x u\|_{H^{m-1}}^2, \quad D_\sigma^m = \|\sigma\|_{H^m}^2 + \|\partial_x \sigma\|_{H^{m-1}}^2.$

To get the regularity of the solution in the Hilbert space, one usually uses energy estimates. In order to balance the nonlinear term $\partial_x \phi \partial_v f$, and get a regularity independent of the small parameter ε (or depending on ε in a good way), one needs the hypocoercivity property from the collision operator. The hypocoercivity property one uses most commonly is

$$-\langle \mathcal{L}^F h, h \rangle \geq C \|(1 - \Pi_1)h\|^2, \quad (50)$$

see [21, 76]. However, this is not enough for the non-linear case. We need the following stronger hypocoercivity (see [22]):

Proposition 1 For \mathcal{L}^F defined in (48),

- (a) $-\langle \mathcal{L}^F h, h \rangle = -\langle L(1 - \Pi)h, (1 - \Pi)h \rangle + \|u\|^2$;
- (b) $-\langle \mathcal{L}^F(1 - \Pi)h, (1 - \Pi)h \rangle = \|\partial_v(1 - \Pi)h\|^2 + \frac{1}{4}\|v(1 - \Pi)h\|^2 - \frac{1}{2}\|(1 - \Pi)h\|^2$;
- (c) $-\langle \mathcal{L}^F(1 - \Pi)h, (1 - \Pi)h \rangle \geq \|(1 - \Pi)h\|^2$;
- (d) There exists a constant $\lambda_0 > 0$, such that the following hypocoercivity holds,

$$-\langle \mathcal{L}^F h, h \rangle \geq \lambda_0 \|(1 - \Pi)h\|_v^2 + \|u\|^2, \quad (51)$$

and the largest $\lambda_0 = \frac{1}{7}$ in one dimension.

The following results were obtained in [43].

Theorem 6 For the high field regime ($\delta = 1$), if

$$E_h^m(0) + \frac{1}{\varepsilon^2} E_\phi^m(0) \leq C_0, \quad (52)$$

then,

$$E_h^m(t) \leq \frac{3}{\lambda_0} e^{-\frac{t}{\varepsilon^2}} \left(E_h^m(0) + \frac{1}{\varepsilon^2} E_\phi^m(0) \right), \quad E_\phi^m(t) \leq \frac{3}{\lambda_0} e^{-t} \left(\varepsilon^2 E_h^m(0) + E_\phi^m(0) \right); \quad (53)$$

For the parabolic regime ($\delta = \varepsilon$), if

$$E_h^m(0) + \frac{1}{\varepsilon} E_\phi^m(0) \leq \frac{C_0}{\varepsilon}, \quad (54)$$

then,

$$E_h^m(t) \leq \frac{3}{\lambda_0} e^{-\frac{t}{\varepsilon}} \left(E_h^m(0) + \frac{1}{\varepsilon} E_\phi^m(0) \right), \quad E_\phi^m(t) \leq \frac{3}{\lambda_0} e^{-t} \left(\varepsilon E_h^m(0) + E_\phi^m(0) \right). \quad (55)$$

Here $C_0 = 2\lambda_0^3/(80AC_1)^2$, $B = 48\sqrt{m} \binom{m}{[m/2]}$ is a constant only depending on m , $[m/2]$ is the smallest integer larger or equal to $\frac{m}{2}$, and C_1 is the Sobolev constant in one dimension, and $m \geq 1$.

These results show that the solution will converge to the global Maxwellian M^v . Since M^v is independent of z , one sees that the impact of the randomness dies out exponentially in time, in both asymptotic regimes.

The above theorem also leads to the following regularity result for the solution to VPPF system:

Theorem 7 *Under the same condition given in Theorem 6, for $x \in [0, l]$, one has*

$$\|f(t)\|_{H_z^m}^2 \leq \frac{3}{\lambda_0} E^m(0) + 2t^2, \quad (56)$$

where $E^m(0) = E_h^m(0) + \frac{1}{\varepsilon^2} E_\phi^m$.

This Theorem shows that the regularity of the initial data in the random space is preserved in time. Furthermore, the bound of the Sobolev norm of the solution is independent of the small parameter ε .

3.5 The Classical Nonlinear Boltzmann Equation

In this subsection, we consider the spatially homogeneous classical Boltzmann equation

$$\partial_t f = \mathcal{Q}^b(f, f) \quad (57)$$

subject to random initial data and random collision kernel

$$f(0, \mathbf{v}, z) = f^0(\mathbf{v}, z), \quad B = B(\mathbf{v}, \mathbf{v}_*, \eta, z), \quad z \in I_z.$$

We define the norms and operators:

$$\|f(t, \cdot, z)\|_{L_v^p} = \left(\int_{\mathbb{R}^d} |f(t, \mathbf{v}, z)|^p d\mathbf{v} \right)^{1/p}, \quad \|f(t, \mathbf{v}, \cdot)\|_{L_z^2} = \left(\int_{I_z} f(t, \mathbf{v}, z)^2 \pi(z) dz \right)^{1/2},$$

$$\|f(t, \cdot, \cdot)\|_k = \sup_{z \in I_z} \left(\sum_{l=0}^k \|\partial_z^l f(t, \mathbf{v}, z)\|_{L_v^2}^2 \right)^{1/2}.$$

$$\mathcal{Q}^b(g, h)(\mathbf{v}) = \int_{\mathbb{R}^d} \int_{S^{d-1}} B(\mathbf{v}, \mathbf{v}_*, \eta, z) [g(\mathbf{v}')h(\mathbf{v}'_*) - g(\mathbf{v})h(\mathbf{v}_*)] d\eta d\mathbf{v}_*.$$

$$\mathcal{Q}_1^b(g, h)(\mathbf{v}) = \int_{\mathbb{R}^d} \int_{S^{d-1}} \partial_z B(\mathbf{v}, \mathbf{v}_*, \eta, z) [g(\mathbf{v}')h(\mathbf{v}'_*) - g(\mathbf{v})h(\mathbf{v}_*)] d\eta d\mathbf{v}_*.$$

The regularity, studied in [34], relies on the following estimates of $\mathcal{Q}^b(g, h)$ and $\mathcal{Q}_1^b(g, h)$, which are standard results in the deterministic case [10, 58] and straightforward extension to the uncertain case:

Lemma 1 *Assume the collision kernel B depends on z linearly, B and $\partial_z B$ are locally integrable and bounded in z . If $g, h \in L^1_\nu \cap L^2_\nu$, then*

$$\|\mathcal{Q}^b(g, h)\|_{L^2_\nu}, \|\mathcal{Q}_1^b(g, h)\|_{L^2_\nu} \leq C_B \|g\|_{L^1_\nu} \|h\|_{L^2_\nu}, \quad (58)$$

$$\|\mathcal{Q}^b(g, h)\|_{L^2_\nu}, \|\mathcal{Q}_1^b(g, h)\|_{L^2_\nu} \leq C_B \|g\|_{L^2_\nu} \|h\|_{L^2_\nu}, \quad (59)$$

where the constant $C_B > 0$ depends only on B and $\partial_z B$.

We state the following theorem proved in [34].

Theorem 8 *Assume that B satisfies the assumption in Lemma 1, and $\sup_{z \in I_z} \|f^0\|_{L^1_\nu} \leq M$, $\|f^0\|_k < \infty$ for some integer $k \geq 0$. Then there exists a constant $C_k > 0$, depending only on C_B, M, T , and $\|f^0\|_k$ such that*

$$\|f\|_k \leq C_k, \quad \text{for any } t \in [0, T]. \quad (60)$$

This result shows that, even for the nonlinear Boltzmann equation, the regularity of the initial data is preserved in time in the random space.

This result can be easily generalized to the full Boltzmann equation (23) with periodic or vanishing boundary condition in space, we omit the detail. Linear dependence of the collision kernel on the random variable can also be relaxed. See [34] for a general proof.

One should notice that if one considers the Euler regime (by putting an ε^{-1} in front of \mathcal{Q}^b , then C_k in (60) will depend on the reciprocal of ε , in addition to being a large k -dependent constant (which is already the case for the deterministic problem [24]). This estimate breaks down in the Euler limit when $\varepsilon \rightarrow 0$.

4 Generalized Polynomial Chaos Based Stochastic Galerkin (gPC-sG) Methods for Random Kinetic Equations

In the last two decades, a large variety of numerical methods have been developed in the field of uncertainty quantification (UQ) [27, 32, 55, 77]. Among these methods, the most popular ones are Monte-Carlo methods [64], stochastic collocation methods [4, 5, 78] and stochastic Galerkin methods [3, 5]. The idea of Monte-Carlo methods is to sample randomly in the random space, which results in halfth order convergence. Stochastic collocation methods use sample points on a well-designed grid, and one can evaluate the statistical moments by numerical quadratures. Stochastic Galerkin methods start from an orthonormal basis in the random space, and approximate functions by truncated polynomial chaos expansions. By the Galerkin projection, a deterministic system of the expansion coefficients can be obtained. While Monte-Carlo methods have advantage in very high dimensional random space, the other two methods can achieve spectral accuracy if one adopts the generalized polynomial chaos (gPC) basis [79], which is a great advantage if

the dimension of the random space is not too high. In this paper we focus on low dimensional random space, and adopt the stochastic Galerkin (sG) approach.

In the gPC expansion, one approximates the solution of a stochastic problem via an orthogonal polynomial series [79] by seeking an expansion in the following form:

$$f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) \approx \sum_{|\mathbf{k}|=0}^M f_{\mathbf{k}}(t, \mathbf{x}, \mathbf{v}) \Phi_{\mathbf{k}}(\mathbf{z}) := f_M(t, \mathbf{x}, \mathbf{v}, \mathbf{z}), \quad (61)$$

where $\mathbf{k} = (k_1, \dots, k_n)$ is a multi-index with $|\mathbf{k}| = k_1 + \dots + k_n$. $\{\Phi_{\mathbf{k}}(\mathbf{z})\}$ are from \mathbb{P}_M^n , the set of all n -variate polynomials of degree up to M and satisfy

$$\langle \Phi_{\mathbf{k}}, \Phi_{\mathbf{j}} \rangle_{\omega} = \int_{I_{\mathbf{z}}} \Phi_{\mathbf{k}}(\mathbf{z}) \Phi_{\mathbf{j}}(\mathbf{z}) \omega(\mathbf{z}) d\mathbf{z} = \delta_{\mathbf{k}\mathbf{j}}, \quad 0 \leq |\mathbf{k}|, |\mathbf{j}| \leq M.$$

Here $\delta_{\mathbf{k}\mathbf{j}}$ is the Kronecker delta function. The orthogonality with respect to $\omega(\mathbf{z})$, the probability density function of \mathbf{z} , then defines the orthogonal polynomials. For example, the Gaussian distribution defines the Hermite polynomials; the uniform distribution defines the Legendre polynomials, etc. Note that when the random dimension $n > 1$, an ordering scheme for multiple index can be used to re-order the polynomials $\{\Phi_{\mathbf{k}}(\mathbf{z}), 0 \leq |\mathbf{k}| \leq M\}$ into a single index $\{\Phi_k(\mathbf{z}), 1 \leq k \leq N_M = \dim(\mathbb{P}_M^n) = \binom{M+n}{M}\}$. Typically, the graded lexicographic order is used, see, for example, Section 5.2 of [77].

Now inserting (61) into a general kinetic equation

$$\begin{cases} \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \nabla_{\mathbf{x}} \phi \cdot \nabla_{\mathbf{v}} f = \mathcal{Q}(f), & t > 0, \mathbf{x} \in \Omega, \mathbf{v} \in \mathbb{R}^d, \mathbf{z} \in I_{\mathbf{z}}, \\ f(0, \mathbf{x}, \mathbf{v}) = f^0(\mathbf{x}, \mathbf{v}), & \mathbf{x} \in \Omega, \mathbf{v} \in \mathbb{R}^d, \mathbf{z} \in I_{\mathbf{z}}, \\ f(t, \mathbf{x}, \mathbf{v}) = g(t, \mathbf{x}, \mathbf{v}), & t \geq 0, \mathbf{x} \in \partial\Omega, \mathbf{v} \in \mathbb{R}^d, \mathbf{z} \in I_{\mathbf{z}}. \end{cases} \quad (62)$$

Upon a standard Galerkin projection, one obtains for each $0 \leq |\mathbf{k}| \leq M$,

$$\begin{cases} \partial_t f_{\mathbf{k}} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_{\mathbf{k}} + \sum_{|\mathbf{j}|=0}^M \nabla_{\mathbf{x}} \phi_{\mathbf{k}\mathbf{j}} \cdot \nabla_{\mathbf{v}} f_{\mathbf{j}} = \mathcal{Q}_{\mathbf{k}}(f_M), & t > 0, \mathbf{x} \in \Omega, \mathbf{v} \in \mathbb{R}^d, \\ f_{\mathbf{k}}(0, \mathbf{x}, \mathbf{v}) = f_{\mathbf{k}}^0(\mathbf{x}, \mathbf{v}), & \mathbf{x} \in \Omega, \mathbf{v} \in \mathbb{R}^d, \\ f_{\mathbf{k}}(t, \mathbf{x}, \mathbf{v}) = g_{\mathbf{k}}(t, \mathbf{x}, \mathbf{v}), & t \geq 0, \mathbf{x} \in \partial\Omega, \mathbf{v} \in \mathbb{R}^d, \end{cases} \quad (63)$$

with

$$\begin{aligned} \mathcal{Q}_{\mathbf{k}}(f_M) &:= \int_{I_{\mathbf{z}}} \mathcal{Q}(f_M)(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \omega(\mathbf{z}) d\mathbf{z}, \quad \phi_{\mathbf{k}\mathbf{j}} := \int_{I_{\mathbf{z}}} \phi(t, \mathbf{x}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \Phi_{\mathbf{j}}(\mathbf{z}) \omega(\mathbf{z}) d\mathbf{z}, \\ f_{\mathbf{k}}^0 &:= \int_{I_{\mathbf{z}}} f^0(\mathbf{x}, \mathbf{v}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \omega(\mathbf{z}) d\mathbf{z}, \quad g_{\mathbf{k}} := \int_{I_{\mathbf{z}}} g(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \omega(\mathbf{z}) d\mathbf{z}. \end{aligned}$$

Here the collision operator $\mathcal{Q}(f_M)$ could be either linear or nonlinear depending on the specific problem. We also assume that the potential $\phi(t, \mathbf{x}, \mathbf{z})$ is given a priori for simplicity (the case that it is coupled to a Poisson equation can be treated similarly).

Therefore, one has a system of *deterministic* equations to solve and the unknowns are gPC coefficients $f_{\mathbf{k}}$, which are independent of \mathbf{z} . Mostly importantly, the resulting gPC-sG system is just a vector analogue of its deterministic counterpart, thus allowing straightforward extension of the existing deterministic kinetic solvers (of course special attention is needed for the collision operator which will be discussed later). Once the coefficients $f_{\mathbf{k}}$ are obtained through some numerical procedure, the statistical information such as the mean, covariance, standard deviation of the true solution f can be approximated as

$$\mathbb{E}[f] \approx f_0, \quad \text{Var}[f] \approx \sum_{|\mathbf{k}|=1}^M f_{\mathbf{k}}^2, \quad \text{Cov}[f] \approx \sum_{|i|,|j|=1}^M f_i f_j.$$

4.1 Property of the Collision Operator Under the gPC-sG Approximation

Due to the truncated approximation (61), the positivity of f is immediately lost. Thus some properties such as the H -theorem no longer holds under the gPC-sG approximation. Yet the conservation of the collision operator, for instance (26), is still valid (whose proof does not require the positivity of f). Normally these need to be analyzed based on the specific collision operator. We give a simple example here (see [40] for the proof).

Lemma 2 *For the semiconductor Boltzmann collision operator (13) with random scattering kernel $\sigma = \sigma(\mathbf{v}, \mathbf{v}_*, \mathbf{z})$, if its gPC-sG approximation $\mathcal{Q}_{\mathbf{k}}^s = 0$ for every $0 \leq |\mathbf{k}| \leq M$, then it admits a unique solution $f_{\mathbf{k}} = \rho_{\mathbf{k}} M^s(\mathbf{v})$, $0 \leq |\mathbf{k}| \leq M$, where $\rho_{\mathbf{k}} := \int_{\mathbb{R}^d} f_{\mathbf{k}} \, d\mathbf{v}$.*

This lemma is just a vector analogue of the property (15).

4.2 An Efficient Treatment of the Boltzmann Collision Operator Under the gPC-sG Approximation

As mentioned previously, numerical discretization of the gPC-sG system (63) for most kinetic equations does not present essential difficulties. In principle, any time and spatial discretization used for the deterministic, scalar kinetic equations can be generalized easily to the vectorized form. However, this is not the case for the collision operator, especially when it is nonlinear. To illustrate the idea, we use the classical Boltzmann collision operator as an example.

Under the gPC-sG approximation, the \mathbf{k} th-mode of the classical Boltzmann collision operator (24) is given by

$$\begin{aligned} Q_{\mathbf{k}}^b(t, \mathbf{x}, \mathbf{v}) &= \int_{I_{\mathbf{z}}} \mathcal{Q}^b(f_M, f_M)(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \omega(\mathbf{z}) d\mathbf{z} \\ &= \sum_{|\mathbf{i}|, |\mathbf{j}|=0}^M S_{\mathbf{kij}} \int_{\mathbb{R}^d} \int_{S^{d-1}} |\mathbf{v} - \mathbf{v}_*|^\lambda [f_{\mathbf{i}}(\mathbf{v}') f_{\mathbf{j}}(\mathbf{v}'_*) - f_{\mathbf{i}}(\mathbf{v}) f_{\mathbf{j}}(\mathbf{v}_*)] d\eta d\mathbf{v}_*, \end{aligned} \quad (64)$$

with

$$S_{\mathbf{kij}} := \int_{I_{\mathbf{z}}} b_\lambda(\mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \Phi_{\mathbf{i}}(\mathbf{z}) \Phi_{\mathbf{j}}(\mathbf{z}) \omega(\mathbf{z}) d\mathbf{z}, \quad (65)$$

where we assumed that the collision kernel takes the form (25) with uncertainty in b_λ .

Note that the tensor $S_{\mathbf{kij}}$ does not depend on the solution $f_{\mathbf{k}}$, so it can be precomputed and stored for repeated use. But even so, the evaluation of $Q_{\mathbf{k}}^b$ still presents a challenge. A naive, direct computation for each t, \mathbf{x} , and \mathbf{k} would result in $O(N_M^2 N_\eta^{d-1} N_v^{2d})$ complexity, where $N_M = \binom{M+n}{M}$ is the dimension of \mathbb{P}_M^n , N_η is the number of discrete points in each angular direction, and N_v is the number of points in each velocity dimension. This is, if not impossible, prohibitively expensive.

In [34], we constructed a fast algorithm for evaluating (64). It was shown that the above direct cost $O(N_M^2 N_\eta^{d-1} N_v^{2d})$ can be reduced to $\max\{O(R_{\mathbf{k}} N_\eta^{d-1} N_v^d \log N_v), O(R_{\mathbf{k}} N_M N_v^d)\}$ with $R_{\mathbf{k}} \leq N_M$ by leveraging the singular value decomposition (SVD) and the fast spectral method for the deterministic collision operator [62]. This is achieved in two steps.

First, for each fixed \mathbf{k} , decompose the symmetric matrix $(S_{\mathbf{kij}})_{N_M \times N_M}$ as (via a truncated SVD with desired accuracy)

$$S_{\mathbf{kij}} = \sum_{r=1}^{R_{\mathbf{k}}} U_{ir}^{\mathbf{k}} V_{rj}^{\mathbf{k}}.$$

Substituting it into (64) and rearranging terms, one gets

$$Q_{\mathbf{k}}^b(\mathbf{v}) = \sum_{r=1}^{R_{\mathbf{k}}} \int_{\mathbb{R}^d} \int_{S^{d-1}} |\mathbf{v} - \mathbf{v}_*|^\lambda [g_r^{\mathbf{k}}(\mathbf{v}') h_r^{\mathbf{k}}(\mathbf{v}'_*) - g_r^{\mathbf{k}}(\mathbf{v}) h_r^{\mathbf{k}}(\mathbf{v}_*)] d\eta d\mathbf{v}_*, \quad (66)$$

with

$$g_r^{\mathbf{k}}(\mathbf{v}) := \sum_{|\mathbf{i}|=0}^M U_{i'r}^{\mathbf{k}} f_{\mathbf{i}}(\mathbf{v}), \quad h_r^{\mathbf{k}}(\mathbf{v}) := \sum_{|\mathbf{j}|=0}^M V_{rj}^{\mathbf{k}} f_{\mathbf{j}}(\mathbf{v}).$$

Hence one readily reduce the cost from $O(N_M^2 N_\eta^{d-1} N_v^{2d})$ to $\max\{O(R_k N_\eta^{d-1} N_v^{2d}), O(R_k N_M N_v^d)\}$, where $R_k \leq N_M$ is the numerical rank of matrix $(S_{\mathbf{k}ij})_{N_M \times N_M}$.

Next, note that (66) can be formally written as

$$Q_{\mathbf{k}}^b(\mathbf{v}) = \sum_{r=1}^{R_k} \mathcal{Q}^b(g_r^{\mathbf{k}}, h_r^{\mathbf{k}}), \quad (67)$$

and \mathcal{Q}^b is the deterministic collision operator (24) with kernel $B = |\mathbf{v} - \mathbf{v}_*|^\lambda$. In [62], a fast Fourier-spectral method in velocity variable \mathbf{v} was developed for (24) in the case of 2D Maxwell molecule ($\lambda = 0$) and 3D hard-sphere molecule ($\lambda = 1$). Applying this method to (67) with slight modification, one can further reduce the cost from $\max\{O(R_k N_\eta^{d-1} N_v^{2d}), O(R_k N_M N_v^d)\}$ to $\max\{O(R_k N_\eta^{d-1} N_v^d \log N_v), O(R_k N_M N_v^d)\}$, see appendix of [34] for a detailed description (in practice, typically $N_\eta \ll N_v$ [23, 25]).

The above method has been extended to the Fokker-Planck-Landau collision operator in [36]. When the random variable is in high dimension, the problem suffers from the dimension curse. A wavelet based sparse grid method was introduced in [70], in which the matrix $(S_{\mathbf{k}ij})_{N_M \times N_M}$ is very sparse, and the computational cost can be significantly reduced.

4.3 A Spectral Accuracy Analysis

The regularity results presented previously can be used to establish the spectral convergence of the gPC-sG method. As in Sect. 3.5, we will restrict to the spatially homogeneous Boltzmann equation (57).

Using the orthonormal basis $\{\Phi_k(z)\}$, the solution f to (57) can be represented as

$$f(t, \mathbf{v}, z) = \sum_{k=0}^{\infty} \hat{f}_k(t, \mathbf{v}) \Phi_k(z), \quad \text{where} \quad \hat{f}_k(t, \mathbf{v}) = \int_{I_z} f(t, \mathbf{v}, z) \Phi_k(z) \omega(z) dz. \quad (68)$$

Let P_M be the projection operator defined as

$$P_M f(t, \mathbf{v}, z) = \sum_{k=0}^M \hat{f}_k(t, \mathbf{v}) \Phi_k(z).$$

Define the norms

$$\begin{aligned} \|f(t, \mathbf{v}, \cdot)\|_{H_z^k} &= \left(\sum_{l=0}^k \|\partial_z^l f(t, \mathbf{v}, z)\|_{L_z^2}^2 \right)^{1/2}, \\ \|f(t, \cdot, \cdot)\|_{L_{\mathbf{v},z}^2} &= \left(\int_{I_z} \int_{\mathbb{R}^d} f(t, \mathbf{v}, z)^2 d\mathbf{v} \omega(z) dz \right)^{1/2}, \end{aligned} \quad (69)$$

then one has the following projection error.

Lemma 3 Assume z obeys uniform distribution, i.e., $z \in I_z = [-1, 1]$ and $\omega(z) = 1/2$ (so $\Phi_k(z)$ are Legendre polynomials). If $\|f^0\|_m$ is bounded, then

$$\|f - P_M f\|_{L^2_{\mathbf{v},z}} \leq \frac{C}{M^m}, \quad (70)$$

where C is a constant.

Given the gPC approximation of f :

$$f_M(t, \mathbf{v}, z) = \sum_{k=0}^M f_k(t, \mathbf{x}, \mathbf{v}) \Phi_k(z), \quad (71)$$

define the error function

$$e_M(t, \mathbf{v}, z) = P_M f(t, \mathbf{v}, z) - f_M(t, \mathbf{v}, z) := \sum_{k=0}^M e_k(t, \mathbf{v}) \Phi_k(z),$$

where $e_k = \hat{f}_k - f_k$. Then we have

Theorem 9 ([34]) Assume the random variable z and initial data f^0 satisfy the assumption in Lemma 3, and the gPC approximation f_M is uniformly bounded in M , then

$$\|f - f_M\|_{L^2_{\mathbf{v},z}} \leq C(t) \left\{ \frac{1}{M^m} + \|e_M(0)\|_{L^2_{\mathbf{v},z}} \right\},$$

where C is a constant depending on t .

Remark 1 Clearly for spectral accuracy, one needs $\|e_M(0)\|_{L^2_{\mathbf{v},z}} \leq C/M^m$. In practice, one chooses $f_k(0, \mathbf{v}) = \hat{f}_k(0, \mathbf{v})$, for all $k = 0, \dots, M$, then $e_M(0) = 0$.

4.4 Numerical Examples

We now show two typical examples of the kinetic equations subject to random inputs. The first one is the classical Boltzmann equation with random boundary condition and the second one is the semiconductor Boltzmann equation with random force field. For simplicity, we assume the random variable z is one-dimensional and obeys uniform distribution.

Example 1 Consider the classical Boltzmann equation (23) with the following boundary condition: the gas is initially in a constant state

$$f^0(x, \mathbf{v}) = \frac{1}{2\pi T^0} e^{-\frac{\mathbf{v}^2}{2T^0}}, \quad T^0 = 1, \quad x \in [0, 1].$$

At time $t = 0$, suddenly increase the wall temperature at left boundary by a factor of 2 with a small random perturbation:

$$T_w(z) = 2(T^0 + sz), \quad s = 0.2.$$

The purely diffusive Maxwell boundary condition is assumed at $x = 0$. For other implementation details, see [34].

The deterministic version of this problem has been considered by many authors [1, 23, 26], where they all observed that with the sudden rise of wall temperature, the gas close to the wall is heated and accordingly the pressure there rises sharply, which pushes the gas away from the wall and a shock wave propagates into the domain. The mean of our solution also exhibits a similar behavior, see Fig. 1. Meanwhile, the standard deviation of the solution allows us to predict the propagation of uncertainties quantitatively.

Example 2 Consider the semiconductor Boltzmann equation (10) coupled with a Poisson equation:

$$\beta(z)\partial_{xx}\phi = \rho - h(x, z), \quad \phi(0) = 0, \quad \phi(1) = 5, \quad x \in [0, 1],$$

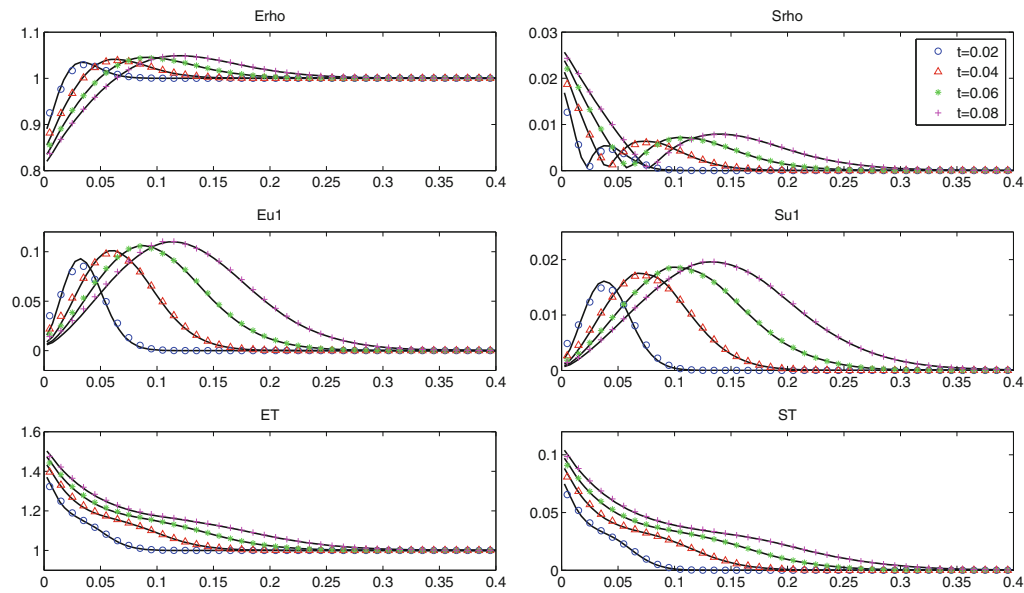


Fig. 1 Example 1. Left column: mean of density, bulk velocity (first component), and temperature. Right column: standard deviation of density, bulk velocity (first component), and temperature. Solid line: stochastic collocation with $N_z = 20$, $N_v = 64$, $N_\eta = 8$, $N_x = 200$. Other legends are the 7-th order gPC-sG solutions at different time with $N_v = 32$, $N_\eta = 4$, $N_x = 100$

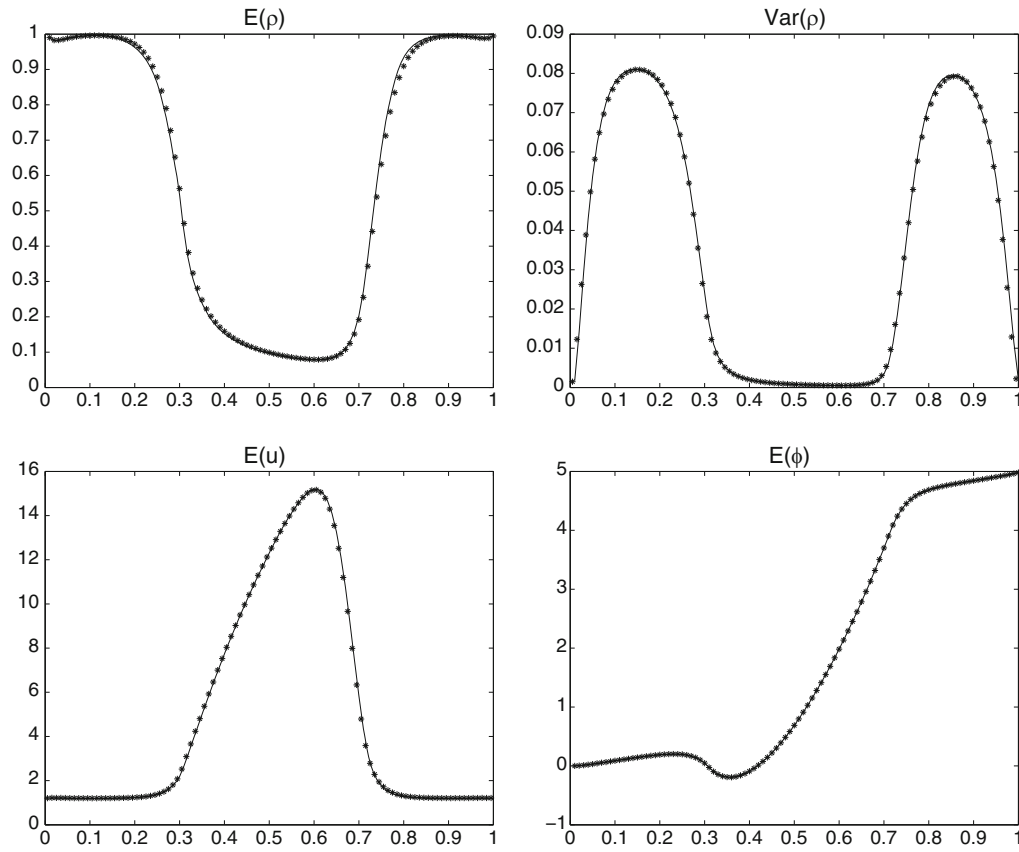


Fig. 2 Example 2. First row: mean and variance of ρ . Second row: mean of velocity u and potential ϕ . Time $t = 0.05$, $\Delta x = 0.01$, $\Delta t = 10^{-5}$, $\varepsilon = 0.001$. Star: 4-th order gPC-sG solutions. Solid line: the reference solutions obtained by stochastic collocation

where we assume the scaled Debye length $\beta(z)$ and the doping profile $h(x, z)$ are subject to uncertainty:

$$\beta(z) = 0.002(1 + 0.2z),$$

$$c(x, z) = \left(1 - (1 - s_0)\rho(0, t = 0) \left[\tanh\left(\frac{x - x_1}{s}\right) - \tanh\left(\frac{x - x_2}{s}\right) \right] \right) (1 + 0.5z),$$

with $s = 0.02$, $s_0 = (1 - 0.001)/2$, $x_1 = 0.3$, $x_2 = 0.7$. For other implementation details, see [40].

The 4-th order gPC solutions and the reference solutions obtained by stochastic collocation are shown in Fig. 2, and they are in good agreement.

5 Stochastic Asymptotic-Preserving (sAP) Schemes for Random Kinetic Equations in Diffusive Scalings

Kinetic equations often have scaling parameters (such as the Knudsen number ε) that asymptotically lead kinetic equations to their hydrodynamic or diffusion limit equations. When ε is small, numerically solving the kinetic equations is challenging since time and spatial discretizations need to resolve ε . Asymptotic-preserving (AP) schemes are those that mimic the asymptotic transitions from kinetic equations to their hydrodynamic/diffusion limits in the discrete setting [35, 37, 38, 53, 54]. Starting from the mid-1990s, the development of AP schemes for such problems has generated many interests, see, for example, [29, 30, 39, 44, 45, 49, 56]. The AP strategy has been proved to be a powerful and robust technique to address multiscale problems in many kinetic problems. The main advantage of AP schemes is that they are very efficient even when ε is small, since they do not need to resolve the small scales numerically, and yet can still capture the macroscopic behavior governed by the limiting macroscopic equations. Indeed, it was proved, in the case of linear transport with a diffusive scaling, an AP scheme converges uniformly with respect to the scaling parameter [29]. This is expected to be true for all AP schemes [38], although specific proofs are needed for specific problems. AP schemes avoid the difficulty of coupling a microscopic solver with a macroscopic one, as the micro solver *automatically* becomes a macro solver as $\varepsilon \rightarrow 0$.

Here we are interested in the scenario when the uncertainty (random inputs) and small scaling both present in a kinetic equation. Since the sG method makes the random kinetic equations into deterministic systems which are vector analogue of the original scalar deterministic kinetic equations, one can naturally utilize the deterministic AP machinery to solve the sG system to achieve the desired AP goals. To this aim, the notion of *stochastic asymptotic preserving (sAP)* was introduced in [46]. A scheme is sAP if a sG method for the random kinetic equation becomes a sG approximation for the limiting macroscopic, random (hydrodynamic or diffusion) equation as $\varepsilon \rightarrow 0$, with highest gPC degree, mesh size and time step all held fixed. Such schemes guarantee that even for $\varepsilon \rightarrow 0$, *all* numerical parameters, including the number of gPC modes, can be chosen only for accuracy requirement and *independent* of ε .

Next we use the linear transport equation (1) as an example to derive a sAP scheme. It has the merit that rigorous convergence and sAP theory can be established, see [47].

5.1 A sAP-sG Method for the Linear Transport Equation

We assume the complete orthogonal polynomial basis in the Hilbert space $H(I_z; \omega(z) dz)$ corresponding to the weight $\omega(z)$ is $\{\phi_i(z), i = 0, 1, \dots, \}$, where

$\phi_i(z)$ is a polynomial of degree i and satisfies the orthonormal condition:

$$\langle \phi_i, \phi_j \rangle_\omega = \int \phi_i(z) \phi_j(z) \omega(z) dz = \delta_{ij}.$$

Here $\phi_0(z) = 1$, and δ_{ij} is the Kronecker delta function. Since the solution $f(t, \cdot, \cdot, \cdot)$ is defined in $L^2([0, 1] \times [-1, 1] \times \mathbb{I}_z; d\mu)$, one has the gPC expansion

$$f(t, x, v, z) = \sum_{i=0}^{\infty} f_i(t, x, v) \phi_i(z), \quad \hat{f} = (f_i)_{i=0}^{\infty} := (\bar{f}, \hat{f}_1).$$

The mean and variance of f can be obtained from the expansion coefficients as

$$\bar{f} = E(f) = \int_{I_z} f \omega(z) dz = f_0, \quad \text{var}(f) = |\hat{f}_1|^2.$$

Denote the sG solution by

$$f_M = \sum_{i=0}^M f_i \phi_i, \quad \hat{f}^M = (f_i)_{i=0}^M := (\bar{f}, \hat{f}_1^M), \quad (72)$$

from which one can extract the mean and variance of f_M from the expansion coefficients as

$$E(f_M) = \bar{f}, \quad \text{var}(f_M) = |\hat{f}_1^M|^2 \leq \text{var}(f).$$

Furthermore, we define

$$\begin{aligned} \sigma_{ij} &= \langle \phi_i, \sigma \phi_j \rangle_\omega, & \Sigma &= (\sigma_{ij})_{M+1, M+1}, \\ \sigma_{ij}^a &= \langle \phi_i, \sigma^a \phi_j \rangle_\omega, & \Sigma^a &= (\sigma_{ij}^a)_{M+1, M+1}, \end{aligned}$$

for $0 \leq i, j \leq M$. Let Id be the $(M+1) \times (M+1)$ identity matrix. Σ, Σ^a are symmetric positive-definite matrices satisfying [77]

$$\Sigma \geq \sigma_{\min} \text{Id}.$$

If one applies the gPC ansatz (72) into the transport equation (1), and conduct the Galerkin projection, one obtains

$$\varepsilon \partial_t \hat{f} + v \partial_x \hat{f} = -\frac{1}{\varepsilon} (I - [\cdot]) \Sigma \hat{f} - \varepsilon \Sigma^a \hat{f} - \hat{S}, \quad (73)$$

where \hat{S} is defined similarly as (72).

We now use the micro-macro decomposition [56]:

$$\hat{f}(t, x, v, z) = \hat{\rho}(t, x, z) + \varepsilon \hat{g}(t, x, v, z), \quad (74)$$

where $\hat{\rho} = [\hat{f}]$ and $[\hat{g}] = 0$, in (73) to get

$$\partial_t \hat{\rho} + \partial_x [v \hat{g}] = -\Sigma^a \hat{\rho} + \hat{S}, \quad (75a)$$

$$\partial_t \hat{g} + \frac{1}{\varepsilon} (I - [\cdot])(v \partial_x \hat{g}) = -\frac{1}{\varepsilon^2} \Sigma \hat{g} - \Sigma^a \hat{g} - \frac{1}{\varepsilon^2} v \partial_x \hat{\rho}, \quad (75b)$$

with initial data

$$\hat{\rho}(0, x, z) = \hat{\rho}_0(x, z), \quad \hat{g}(0, x, v, z) = \hat{g}_0(x, v, z).$$

It is easy to see that system (75) formally has the diffusion limit as $\varepsilon \rightarrow 0$:

$$\partial_t \hat{\rho} = \partial_x (K \partial_x \hat{\rho}) - \Sigma^a \hat{\rho} + \hat{S}, \quad (76)$$

where

$$K = \frac{1}{3} \Sigma^{-1}. \quad (77)$$

This is the sG approximation to the random diffusion equation (8)–(9). Thus the gPC approximation is sAP in the sense of [46].

One can easily derive the following energy estimate for system (75)

$$\begin{aligned} & \int_0^1 \hat{\rho}(t, x)^2 dx + \frac{\varepsilon^2}{2} \int_0^1 \int_{-1}^1 \hat{g}(t, x, v)^2 dv dx \\ & \leq \int_0^1 \hat{\rho}(0, x)^2 dx + \frac{\varepsilon^2}{2} \int_0^1 \int_{-1}^1 \hat{g}(0, x, v)^2 dv dx. \end{aligned}$$

Let f be the solution to the linear transport equation (1)–(2). Use the M th order projection operator P_M , the error arisen from the gPC-sG can be split into two parts r_N and e_N ,

$$f - f_M = f - P_M f + P_M f - f_M := r_M + e_M, \quad (78)$$

where $r_M = f - P_M f$ is the truncation error, and $e_M = P_M f - f_M$ is the projection error.

Here we summarize the results of [47].

Lemma 4 (Truncation Error) *Under all the assumption in Theorems 1 and 2, we have for $t \in (0, T]$ and any integer $k = 0, \dots, m$,*

$$\|r_M\|_r \leq \frac{C_1}{M^k}. \quad (79)$$

Moreover,

$$\| [r_M] - r_M \|_\Gamma \leq \frac{C_2}{M^k} \varepsilon, \quad (80)$$

where C_1 and C_2 are independent of ε .

Lemma 5 (Projection Error) *Under all the assumptions in Theorems 1 and 2, we have for $t \in (0, T]$ and any integer $k = 0, \dots, m$,*

$$\| e_M \|_\Gamma \leq \frac{C(T)}{M^k}, \quad (81)$$

where $C(T)$ is a constant independent of ε .

Combining the above lemmas gives the uniform (in ε) convergence theorem:

Theorem 10 *If for some integer $m \geq 0$,*

$$\| \sigma(z) \|_{H^k} \leq C_\sigma, \quad \| D^k f_0 \|_\Gamma \leq C_0, \quad \| D^k (\partial_x f_0) \|_\Gamma \leq C_x, \quad k = 0, \dots, m, \quad (82)$$

then the error of the sG method is

$$\| f - f_M \|_\Gamma \leq \frac{C(T)}{M^k}, \quad (83)$$

where $C(T)$ is a constant independent of ε .

Theorem 10 gives a uniformly in ε spectral convergence rate, thus one can choose M independent of ε , a very strong sAP property. Such a result is also obtained with the anisotropic scattering case, for the linear semiconductor Boltzmann equation (10) [59].

5.2 A Full Discretization

As pointed out in [46], and also seen in Sect. 4, by using the gPC-sG formulation, one obtains a vector version of the original deterministic transport equation. This enables one to use the deterministic AP methodology. In this paper, we adopt the micro-macro decomposition based AP scheme developed in [56] for the gPC-sG system (75).

We take a uniform grid $x_i = ih, i = 0, 1, \dots, N$, where $h = 1/N$ is the grid size, and time steps $t^n = n\Delta t$. ρ_i^n is the approximation of ρ at the grid point (x_i, t^n) while $g_{i+\frac{1}{2}}^{n+1}$ is defined at a staggered grid $x_{i+\frac{1}{2}} = (i + 1/2)h, i = 0, \dots, N - 1$.

The fully discrete scheme for the gPC system (75) is

$$\frac{\hat{\rho}_i^{n+1} - \hat{\rho}_i^n}{\Delta t} + \left[v \frac{\hat{g}_{i+\frac{1}{2}}^{n+1} - \hat{g}_{i-\frac{1}{2}}^{n+1}}{\Delta x} \right] = -\Sigma_i^a \hat{\rho}_i^{n+1} + \hat{S}_i, \quad (84a)$$

$$\begin{aligned} \frac{\hat{g}_{i+\frac{1}{2}}^{n+1} - \hat{g}_{i+\frac{1}{2}}^n}{\Delta t} + \frac{1}{\varepsilon \Delta x} (I - [\cdot]) \left(v^+ (\hat{g}_{i+\frac{1}{2}}^n - \hat{g}_{i-\frac{1}{2}}^n) + v^- (\hat{g}_{i+\frac{3}{2}}^n - \hat{g}_{i+\frac{1}{2}}^n) \right) \\ = -\frac{1}{\varepsilon^2} \Sigma_i \hat{g}_{i+\frac{1}{2}}^{n+1} - \Sigma^a \hat{g}_{i+\frac{1}{2}}^{n+1} - \frac{1}{\varepsilon^2} v \frac{\hat{\rho}_{i+1}^n - \hat{\rho}_i^n}{\Delta x}. \end{aligned} \quad (84b)$$

It has the formal diffusion limit when $\varepsilon \rightarrow 0$ given by

$$\frac{\hat{\rho}_i^{n+1} - \hat{\rho}_i^n}{\Delta t} - K \frac{\hat{\rho}_{i+1}^n - 2\hat{\rho}_i^n + \hat{\rho}_{i-1}^n}{\Delta x^2} = -\Sigma_i^a \hat{\rho}_i^{n+1} + \hat{S}_i, \quad (85)$$

where $K = \frac{1}{3} \Sigma^{-1}$. This is the fully discrete sG scheme for (76). Thus the fully discrete scheme is sAP.

One important property for an AP scheme is to have a stability condition independent of ε , so one can take $\Delta t \gg O(\varepsilon)$. The next theorem from [47] answers this question.

Theorem 11 Assume $\sigma^a = S = 0$. If Δt satisfies the following CFL condition

$$\Delta t \leq \frac{\sigma_{\min}}{3} \Delta x^2 + \frac{2\varepsilon}{3} \Delta x, \quad (86)$$

then the sequences $\hat{\rho}^n$ and \hat{g}^n defined by scheme (84) satisfy the energy estimate

$$\Delta x \sum_{i=0}^{N-1} \left((\hat{\rho}_i^n)^2 + \frac{\varepsilon^2}{2} \int_{-1}^1 (\hat{g}_{i+\frac{1}{2}}^n)^2 dv \right) \leq \Delta x \sum_{i=0}^{N-1} \left((\hat{\rho}_i^0)^2 + \frac{\varepsilon^2}{2} \int_{-1}^1 (\hat{g}_{i+\frac{1}{2}}^0)^2 dv \right)$$

for every n , and hence the scheme (84) is stable.

Since the right hand side of (86) has a lower bound when $\varepsilon \rightarrow 0$ (and the lower bound being that of a stability condition of the discrete diffusion equation (85)), the scheme is asymptotically stable and Δt remains finite even if $\varepsilon \rightarrow 0$.

A discontinuous Galerkin method based sAP scheme for the same problem was developed in [17], where uniform stability and rigorous sAP property were also proven.

5.3 Numerical Examples

We now show one example from [47] to illustrate the sAP properties of the scheme. For simplicity, we again assume the random variable z is one-dimensional and obeys uniform distribution.

Example 3 Consider the linear transport equation (1) with $\sigma^a = S = 0$ and random coefficient

$$\sigma(z) = 2 + z,$$

subject to zero initial condition $f(0, x, v, z) = 0$ and boundary condition

$$f(t, 0, v, z) = 1, \quad v \geq 0; \quad f(t, 1, v, z) = 0, \quad v \leq 0.$$

When $\varepsilon \rightarrow 0$, the limiting random diffusion equation is

$$\partial_t \rho = \frac{1}{3\sigma(z)} \partial_{xx} \rho, \quad (87)$$

with initial and boundary conditions:

$$\rho(0, x, z) = 0, \quad \rho(t, 0, z) = 1, \quad \rho(t, 1, z) = 0.$$

The analytical solution for (87) with the given initial and boundary conditions is

$$\rho(t, x, z) = 1 - \operatorname{erf} \left(\frac{x}{\sqrt{\frac{4}{3\sigma(z)} t}} \right). \quad (88)$$

When ε is small, we use this as the reference solution, as it is accurate with an error of $O(\varepsilon^2)$. For other implementation details, see [47].

In Fig. 3, we plot the errors in mean and standard deviation of the gPC numerical solutions at $t = 0.01$ with different gPC orders M . Three sets of results are included: solutions with $\Delta x = 0.04$ (squares), $\Delta x = 0.02$ (circles), $\Delta x = 0.01$ (stars). We always use $\Delta t = 0.0002/3$. One observes that the errors become smaller with finer mesh. One can see that the solutions decay rapidly in M and then saturate where spatial discretization error dominates. It is then obvious that the errors due to gPC expansion can be neglected at order $M = 4$ even for $\varepsilon = 10^{-8}$. From this simple example, we can see that using the properly designed sAP scheme, the time, spatial, and random domain discretizations can be chosen independently of the small parameter ε .

In Fig. 4, we examine the difference between the solution at $t = 0.01$ obtained by the 4th-order gPC method with $\Delta x = 0.01$, $\Delta t = \Delta x^2/12$ and the limiting analytical solution (88). As expected, we observe the differences become smaller as ε is smaller in a quadratic fashion, before the numerical errors become dominant. This, on the other hand, shows the sAP scheme works uniformly for different ε .

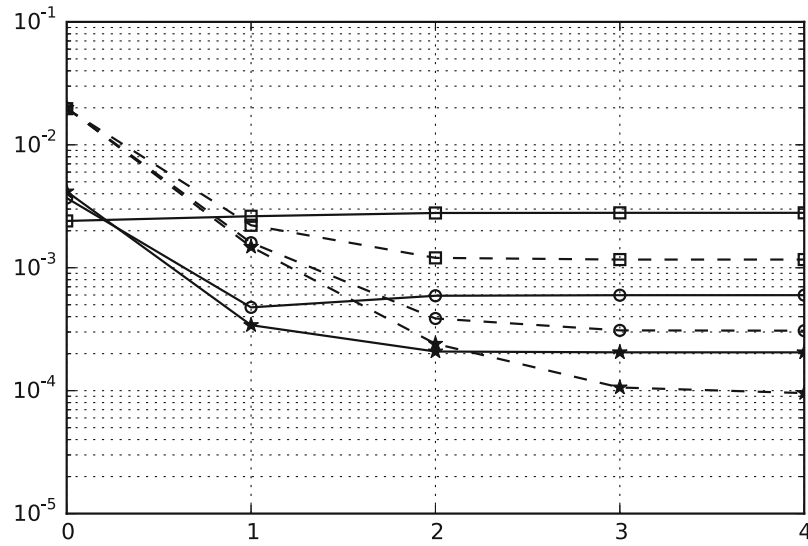


Fig. 3 Example 3. Errors of the mean (solid line) and standard deviation (dash line) of ρ with respect to the gPC order M at $\varepsilon = 10^{-8}$: $\Delta x = 0.04$ (squares), $\Delta x = 0.02$ (circles), $\Delta x = 0.01$ (stars). $\Delta t = 0.0002/3$

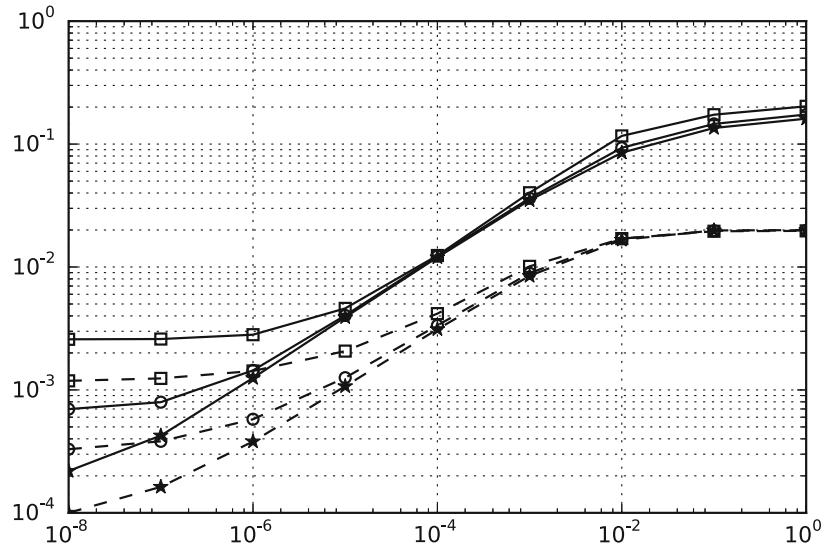


Fig. 4 Example 3. Differences in the mean (solid line) and standard deviation (dash line) of ρ with respect to ε^2 , between the limiting analytical solution (88) and the 4th-order gPC solution with $\Delta x = 0.04$ (squares), $\Delta x = 0.02$ (circles) and $\Delta x = 0.01$ (stars)

6 Conclusion and Open Problems

Using the classical Boltzmann equation, linear Boltzmann equations and Vlasov-Poisson-Fokker-Planck system as prototype examples, we have surveyed recent development of uncertainty quantification (UQ) for kinetic equations. The

uncertainties for such equations typically come from collision/scattering kernels, boundary data, initial data, forcing terms, among others. We proved the regularity in the random space and then adopted the generalized polynomial chaos based stochastic Galerkin (gPC-sG) approach to handle the random inputs which could yield spectral accuracy, under some regularity assumption on the initial data and random coefficients. Various theoretical and computational issues with respect to the collision operator were studied. When the kinetic equation has diffusive scaling that asymptotically leads to a diffusion equation, we constructed the stochastic Asymptotic-Preserving (sAP) scheme which allows numerical discretization including the gPC order to be chosen independently of the small parameter, hence is highly efficient in diffusive regime.

UQ for kinetic equations is a fairly recent research field, and many interesting problems remain open. We list a few such problems here:

- Nonlinear kinetic equations. Although sG or sAP schemes have been introduced for some nonlinear kinetic equations, for example the Boltzmann equation [34], the Landau equation [36], the radiative heat transfer equations [41], disperse two-phase kinetic-fluid model [42], rigorous analysis—such as regularity, long-time and small ε behavior, spectral convergence, etc.—has been lacking. In particular, for the Boltzmann equation, the behavior of the sG scheme in the Euler regime is not understood.
- High dimensional random space. When the dimension of the random parameter \mathbf{z} is moderate, sparse grids have been introduced [36, 70] using wavelet approximations. Since wavelet basis does not have high order accuracy, it remains to construct sparse grids with high (or spectral) order of accuracy in the random space. When the random dimension is much higher, new methods need to be introduced to reduce the dimension.
- Study of sampling based methods such as collocation and multi-level Monte-Carlo methods. In practice, sampling based non-intrusive methods are attractive since they are based on the deterministic, or legacy codes. So far there has been no analysis done for the stochastic collocation methods for random kinetic equations. Moreover, multi-level Monte-Carlo method could significantly reduce the cost of sampling based methods [28]. Its application to kinetic equations with uncertainty remains to be investigated.

Despite at its infancy, due to the good regularity and asymptotic behavior in the random space for kinetic equations with uncertain random inputs, the UQ for kinetic equations is a promising research direction that deserves more development in their mathematical theory, efficient numerical methods, and applications. Moreover, since the random parameters in uncertain kinetic equations share some properties of the velocity variable for a kinetic equation, the ideas from kinetic theory can be very useful for UQ [18], and vice versa, thus the marriage of the two fields can be very fruitful.

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