

ENOC 2017 Extended Abstract

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Summary. I am intended to present my joint paper with Prof Shi Jin, from math department of University of Wisconsin-Madison, USA. We develop a generalized polynomial chaos approach based stochastic Galerkin (gPC-SG) method for the linear semi-conductor Boltzmann equation with random inputs and diffusive scalings. The random inputs are due to uncertainties in the collision kernel or initial data. We study the regularity (uniform in the Knudsen number) of the solution in the random space, and prove the spectral accuracy of the gPC-SG method. We then use the asymptotic-preserving framework for the deterministic counterpart to come up with the stochastic asymptotic-preserving gPC-SG method for the problem under study which is efficient in the diffusive regime. Numerical results will be shown to validate the accuracy and asymptotic properties of the method.

Outline

In the first part of the talk, I will review the idea of asymptotic preserving (AP) schemes for multiscale kinetic equations. One of the challenges in numerical approximations of kinetic and transport equations arise from varying magnitude of the Knudsen number, which is the dimensionless mean free path measuring the ratio between the particle mean free path and a typical length scale. When the Knudsen number is small the equation becomes numerically stiff thus demand prohibitive, Knudsen number dependent mesh sizes and time steps.

To overcome this difficulty, asymptotic-preserving (AP) schemes, which mimic the asymptotic transition from the kinetic equations to the hydrodynamic or diffusion limit, combined with efficient time integrators, have proved to be very efficient to handle small or multiple scales in kinetic or hyperbolic problems, see [2, 3]. The idea of AP schemes can be illustrated in the figure below. For linear transport equations with diffusive scales and random inputs, stochastic asymptotic-preserving (s-AP) schemes were recently introduced in [5]. A s-AP scheme allows the use of mesh sizes, time steps and the number of terms in the orthogonal polynomial expansions *independent of* the Knudsen number, yet can still capture the solution of the limiting, macroscopic equations.

In the second part of the talk, I plan to discuss about the fundamental things for generalized polynomial chaos (gPC) method to deal with uncertainty quantification problems. The random inputs arise in the collision kernel, initial or boundary data due to modeling or measurement errors, which are typical for kinetic equations that are often derived via mean-field limits from particle systems. In recent years there have been significant interests in uncertainty quantification for physical models that contain uncertain coefficients, but few works have been concentrated on kinetic equations which are of practical importance in mesoscopic modeling of physical, biological to social sciences. The idea of the stochastic Galerkin method is seeking for an orthogonal polynomial expansion for the solution. For random variable $\mathbf{z} \in I_{\mathbf{z}}$,

$$f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) \approx f_K(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) = \sum_{|\mathbf{k}|=1}^K \alpha_{\mathbf{k}}(t, \mathbf{x}, \mathbf{v}) \psi_{\mathbf{k}}(\mathbf{z}) = \boldsymbol{\alpha} \cdot \boldsymbol{\psi}, \quad K = \binom{n+P}{n}. \quad (0.1)$$

Here $\mathbf{k} = (k_1, \dots, k_n)$ is a multi-index with $|\mathbf{k}| = k_1 + \dots + k_n$, and the coefficient vectors are given by

$$\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_K), \quad \boldsymbol{\psi} = (\psi_1, \dots, \psi_K).$$

$\{\Psi_{\mathbf{k}}(\mathbf{z})\}$ are the orthonormal basis functions that form \mathbb{P}_P^n (the set of n -variate orthonormal polynomials of degree up to $P \geq 1$) and satisfy

$$\int_{I_{\mathbf{z}}} \psi_{\mathbf{k}}(\mathbf{z}) \psi_{\mathbf{l}}(\mathbf{z}) \pi(\mathbf{z}) d\mathbf{z} = \delta_{\mathbf{k}\mathbf{l}}, \quad 0 \leq |\mathbf{k}|, |\mathbf{l}| \leq K = \dim(\mathbb{P}_P^n),$$

where $\delta_{\mathbf{k}\mathbf{l}}$ the Kronecker Delta function.

$$\begin{array}{ccc} \mathcal{F}_{\delta}^{\varepsilon} & \xrightarrow{\varepsilon \rightarrow 0} & \mathcal{F}_{\delta}^0 \\ \downarrow \delta \rightarrow 0 & & \downarrow \delta \rightarrow 0 \\ \mathcal{F}^{\varepsilon} & \xrightarrow{\varepsilon \rightarrow 0} & \mathcal{F}^0 \end{array}$$

In the last part of the talk, a linear semiconductor Boltzmann equation with random inputs and diffusive scalings will be discussed, namely

$$\begin{cases} \epsilon \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q}{m} \nabla_{\mathbf{x}} \phi(t, \mathbf{x}, \mathbf{z}) \cdot \nabla_{\mathbf{v}} f = \frac{1}{\epsilon} \mathcal{Q}(f)(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) + \epsilon G(t, \mathbf{x}, \mathbf{v}, \mathbf{z}), \\ t > 0, \mathbf{x} \in \Omega \subseteq \mathbb{R}^N, \mathbf{v} \in \mathbb{R}^d, \mathbf{z} \in I_{\mathbf{z}}, \\ f(0, \mathbf{x}, \mathbf{v}, \mathbf{z}) = f_I(\mathbf{x}, \mathbf{v}, \mathbf{z}), \\ f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) = g(t, \mathbf{x}, \mathbf{v}, \mathbf{z}), \quad \mathbf{x} \in \partial\Omega, \quad \mathbf{v} \cdot \mathbf{n} \leq 0. \end{cases} \quad (0.2)$$

$f(t, \mathbf{x}, \mathbf{v}, \mathbf{z})$ is the probability density distribution for particles at $\mathbf{x} \in \Omega$, with velocity $\mathbf{v} \in \mathbb{R}^d$. \mathbf{n} is the unit outer normal vector to the boundary $\partial\Omega$ of the spatial domain, ϵ is the Knudsen number, $\phi(t, \mathbf{x}, \mathbf{z})$ is the electric potential and $\mathbf{E}(t, \mathbf{x}, \mathbf{z}) = -\nabla_{\mathbf{x}} \phi(t, \mathbf{x}, \mathbf{z})$ is the electric field. The constants q and m are respectively the elementary charge and the effective mass of the electron.

The random inputs can come from the collision kernel, electric potential, initial or boundary data. Our method is based on the generalized polynomial chaos approach in the stochastic Galerkin (hereafter referred to as the gPC-SG) framework [1, 6, 7]. The advantage of the gPC-SG method over the classical Monte-Carlo method is that the former enjoys a spectral accuracy in the random space—provided sufficient regularity of the solution—while the latter converges with only half-th order accuracy. The *uniform* regularity of the solution in the random space is studied and the spectral accuracy of the gPC-based stochastic Galerkin (gPC-SG) method is proved, which is summarized in the following theorem.

Theorem 0.1. (Spectral convergence) Assume that σ depends on z linearly, $\hat{\phi} = \|\frac{\partial \phi}{\partial t}\|_{L^\infty(\Omega \times (0, \infty))}$ is bounded, the initial data satisfies $\|f_I\|_{\hat{\mathbf{H}}^m(0)} \leq \beta_1$, and

$$\max_z |\sigma| \leq \gamma_0, \quad \max_z |\partial_z \sigma| \leq \gamma_1,$$

we have

$$\|f - f_K\|_{\Gamma(t)} \leq \frac{C_2}{\epsilon^2} \frac{1}{K^m} \exp \left\{ \left(\hat{\phi} + 2 \frac{\gamma_0 + \gamma_1 m}{\epsilon^2} \right) t \right\}, \quad (0.3)$$

where C_2 is independent of ϵ and m .

We use the asymptotic-preserving framework and the deterministic counterpart for the problem [4] to come up with a stochastic asymptotic-preserving gPC-SG approach that is efficient in the diffusive regime. Numerical examples will be shown to validate the accuracy and asymptotic properties of the method.

References

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