Monte Carlo Stochastic Galerkin methods for the Boltzmann equation

Lorenzo Pareschi

Department of Mathematics and Computer Science
University of Ferrara, Italy

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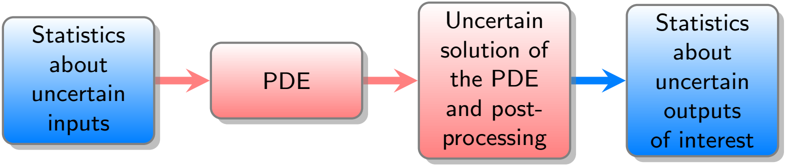
Mattia Zanella, University of Pavia, Italy

Uncertainty quantification for PDEs



- The recent interest in UQ for PDEs can be attributed mainly to three factors:
  - widespread availability of data resulting from advances in technology;
  - increased development of HPC;
  - construction and analysis of new algorithms.
- In presence of uncertainties it becomes necessary to quantify these effects on some quantity of interest (a quantity that depends on the solution of the PDE for which we want to know some statistical information).
- The UQ task then consists of determining information about the uncertainty in an output of interest that depends on the solution of a PDE, given information about the uncertainty in the inputs of the PDE.

Uncertainty in Boltzmann-type equations

Let us focus on the case of kinetic equations of Boltzmann-type

$$\partial_t f(z,x,v,t) + v\cdot\nabla_x f(z,x,v,t) = \frac{1}{\varepsilon} Q(f,f)(z,x,v,t), \qquad (x,v)\in\mathbb{R}^{d_x}\times\mathbb{R}^{d_v},$$

with $\varepsilon > 0$ the Knudsen number and $z\in\Omega\subseteq\mathbb{R}^{d_z}$ a random vector $\sim p(z)$.

In the case of the Boltzmann collision operator we have

$$Q(f,f)(z,x,v,t) = \int_{\mathbb{S}^{d_v-1}\times\mathbb{R}^{d_v}} B(z,v,v_*,\omega)(f(v')f(v'_*)_* - f(v)f(v_*))\,dv_*\,d\omega.$$

where

$$v' = \frac{v+v_*}{2} + \frac{|v-v_*|}{2}\omega, \qquad v'_* = \frac{v+v_*}{2} - \frac{|v-v_*|}{2}\omega.$$

The kernel $B(z,|v-v_*|,\omega)\geqslant 0$ is assumed in the form

$$B(z,v,v_*,\omega) = b_\alpha(z,\omega)|v-v_*|^\alpha.$$

For $\alpha = 0$ we have the Maxwellian case whereas for $\alpha = 1$ the hard sphere case.

Uncertainty quantification

- Stochastic Galerkin methods based on the use of deterministic methods in the phase space[1]. Such methods have demonstrated numerical and theoretical evidence of spectral accuracy. Their computational cost is high due to the curse of dimensionality, the main physical properties of the solution, among which its positivity, are lost.
- Multifidelity methods based on the use of control variate techniques[2]. These methods, are more efficient than Galerkin's stochastic approaches, especially for problems with high dimensionality of the random space. Their non-intrusive nature permits to preserve the physical properties of the underlying deterministic numerical methods in the phase space.
- DSMC stochastic Galerkin methods combine the efficiency of DSMC techniques for the Boltzmann equation in phase space with the accuracy of stochastic Galerkin methods in random space[3]. This novel hybrid formulation makes it possible to construct efficient methods that preserve the main physical properties along with spectral accuracy in the random space.

[1] S.Jin, J.Hu, L.Liu, R.Shu, Y.Zhu, ..., '16-'20

[2] G.Dimarco, L.Pareschi, '19-'20, L.Liu, X.Zhu '20

[3] Similar approach for mean-field problems in J.Carrillo, L.Pareschi, M.Zanella '18-'19

DSMC method for VHS

Let us first consider the deterministic case for variable hard spheres (VHS)

$$B(z, v, v_*, \omega) = B(|v - v_*|).$$

We denote by $Q_\Sigma(f, f)$ the collision operator with the kernel

$$B_\Sigma(|v - v_*|) = \min\{B(|v - v_*|), \Sigma\}, \quad \Sigma > 0.$$

Thus, for a fixed Σ, let us consider the homogeneous problem

$$\frac{\partial f}{\partial t} = Q_\Sigma(f, f) = P(f, f) - \mu f,$$

where the operator $Q_\Sigma(f, f)$ can be written in the form $P(f, f) - \mu f$ taking

$$P(f, f) = Q_\Sigma^+(f, f) + f(v) \int_{\mathbb{R}^{d_v}} \int_{S^{d_v - 1}} [\Sigma - B_\Sigma(|v - v_*|)] f(v_*) \, d\omega \, dv_*,$$

with $\mu = 2^{d_v - 1}\pi\Sigma$ and $Q_\Sigma^+(f, f)$ the gain part of $Q_\Sigma(f, f)$.

Nambu DSMC scheme

To introduce the DSMC scheme we consider a simulation algorithm based on the time discrete form of the above problem originally proposed by Nambu[4].

Consider a time interval $[0, t_{\max}]$, and set $\Delta t = t_{\max}/n_t$. We denote by $f^n(v)$ an approximation of $f(v, n\Delta t)$. The forward Euler scheme reads

$$f^{n+1} = (1 - \mu\Delta t)\, f^n + \mu\Delta t \frac{P(f^n, f^n)}{\mu}.$$

Clearly if f^n is a probability density both $P(f^n, f^n)/\mu$ and f^{n+1} are probability densities provided that $\mu\Delta t \leqslant 1$.

The DSMC scheme is obtained by using the acceptance-rejection technique to sample the post collisional velocity according to $P(f, f)/\mu$. This amounts in computing a Maxwellian collision process (dummy collision) with kernel Σ between v and v_* and in accepting the collision with probability

$$\frac{B_\Sigma(|v - v_*|)}{\Sigma} \leqslant 1.$$

[4] K. Nambu '83, H. Babovski '86

Nanbu-Babovski DSMC algorithm

1. Compute the initial velocities $\{v_i^0, i = 1, \dots, N\}$ sampling from $f_0(v)$
2. for $n = 0$ to $n_t - 1$
   - compute an upper bound Σ of the cross section
   - set $\mu = 2^{d-1}\pi\Sigma$ and $N_c = \text{Sround}(\mu N \Delta t/2)$
   - select N_c dummy collision pairs (i, j) uniformly among all possible pairs, and for those
     - compute the relative cross section $B_{ij} = B(|v_i - v_j|)$
     - if $\Sigma\,\xi < B_{ij}$, ξ uniform in $(0, 1)$
       perform the collision between i and j, and compute
       v_i' and v_j' according to the collision law
       set $v_i^{n+1} = v_i'$, $v_j^{n+1} = v_j'$
   - set $v_i^{n+1} = v_i^n$ for all the particles that have not been selected

   end for

Here by Sround(x) we denote the stochastic rounding of a positive real number x

$$\text{Sround}(x) = \begin{cases} \lfloor x \rfloor + 1 & \text{with probability} \quad x - \lfloor x \rfloor \\ \lfloor x \rfloor & \text{with probability} \quad 1 - x + \lfloor x \rfloor \end{cases}$$

where $\lfloor x \rfloor$ denotes the integer part of x.

Reformulation of DSMC for VHS with uncertainty

In the sequel we will consider

$$B(z, v, v_*, \omega) = B(z, |v - v_*|),$$

and denote by $Q_\Sigma(f, f)$ the collision operator with the kernel

$$B_\Sigma(z, |v - v_*|) = \min\{B(z, |v - v_*|), \Sigma\}, \quad \Sigma > 0.$$

Given a random number ξ uniform in $(0, 1)$, we rewrite the acceptance-rejection collision process in the equivalent form

$$v_i'(z,t) = v_i(z,t) - \frac{1}{2}\Psi(\Sigma\,\xi < B_{ij}(z))\left((v_i(z,t) - v_j(z,t)) - |v_i(z,t) - v_j(z,t)|\omega\right),$$
$$v_j'(z,t) = v_j(z,t) + \frac{1}{2}\Psi(\Sigma\,\xi < B_{ij}(z))\left((v_i(z,t) - v_j(z,t)) - |v_i(z,t) - v_j(z,t)|\omega\right),$$

where $\Psi(\cdot)$ is the indicator function and

$$B_{ij}(z) = B(z, |v_i(z,t) - v_j(z,t)|).$$

Stochastic Galerkin approximation

We consider a set of N samples $v_i(z,t)$, $i = 1, \dots, N$ and approximate $v_i(z,t)$ by its generalized polynomial chaos (gPC) expansion

$$v_i^M(z,t) = \sum_{m=0}^{M} \hat{v}_{i,m}(t)\Phi_m(z).$$

In the above expansion $\{\Phi_m(z)\}_{m=0}^M$ are a set of orthogonal polynomials, of degree less or equal to M orthonormal with respect to the PDF $p(z)$

$$\int_\Omega \Phi_n(z)\Phi_m(z)p(z)\,dz = \mathbb{E}[\Phi_m(\cdot)\Phi_n(\cdot)] = \delta_{mn}, \qquad m,n = 0,\dots,M,$$

and $\hat{v}_{i,m}$ is the projection of the solution with respect to Φ_m

$$\hat{v}_{i,m}(t) = \int_\Omega v_i(z,t)\Phi_m(z)p(z)\,dz = \mathbb{E}[v_i(\cdot,t)\Phi_m(\cdot)].$$

To define the DSMC-sG algorithm we consider the projection on the above space of the collision process in the DSMC method.

Thanks to the new formulation, we can perform the projection on the space of modes in the gPC expansion to get for $m = 0, \dots, M$

$$
\begin{aligned}
\hat{v}'_{i,m}(t) &= \hat{v}_{i,m}(t) - \frac{1}{2}\hat{W}^m_{ij}(\xi, t) + \frac{1}{2}\hat{V}^m_{ij}(\xi, t)\,\omega, \\
\hat{v}'_{j,m}(t) &= \hat{v}_{j,m}(t) + \frac{1}{2}\hat{W}^m_{ij}(\xi, t) - \frac{1}{2}\hat{V}^m_{ij}(\xi, t)\,\omega,
\end{aligned}
$$

where

$$
\begin{aligned}
\hat{W}^m_{ij}(\xi, t) &= \int_\Omega \Psi(\Sigma\,\xi < B_{ij}(z))\left(v_i^M(z, t) - v_j^M(z, t)\right)\Phi_m(z)p(z)\,dz, \\
\hat{V}^m_{ij}(\xi, t) &= \int_\Omega \Psi(\Sigma\,\xi < B_{ij}(z))|v_i^M(z, t) - v_j^M(z, t)|\Phi_m(z)p(z)\,dz.
\end{aligned}
$$

The above quantities are computed at each collision for a given i, j and ξ. Using Gaussian quadrature with H points these can be computed at a cost $O(MH)$. The Maxwellian case is particularly simple, $\Psi = 1$, and reduces the cost to $O(M)$.

DSMC-sG algorithm

1. Compute the initial gPC expansions $\{v_i^{M,0}, i = 1, \ldots, N\}$ from $f_0(v)$
2. for $n = 0$ to $n_t - 1$
   - compute an upper bound Σ of the cross section
   - set $\mu = 2^{d-1}\pi\Sigma$ and $N_c = \text{Sround}(\mu N \Delta t/2)$
   - select N_c dummy collision pairs (i, j) uniformly among all possible pairs and for those
     - Compute the collision matrices $\hat{W}_{ij}^m(\xi)$, $\hat{V}_{ij}^m(\xi)$, $i, j = 1, \ldots, N$, $m = 0, \ldots, M$, ξ uniform in $(0, 1)$.
     - evaluate the collision between i and j, computing $\hat{v}'_{i,m}$ and $\hat{v}'_{j,m}$
     - set $\hat{v}_{i,m}^{n+1} = \hat{v}'_i$, $\hat{v}_{j,m}^{n+1} = \hat{v}'_{j,m}$
   - set $\hat{v}_{i,m}^{n+1} = \hat{v}_{i,m}^n$ for all the particles that have not been selected

end for

Consistency estimate on moments

Given a function $f(z, v, t)$ approximated by Monte Carlo samples, its empirical measure and the empirical measure in the sG representation as

$$f^N(z, v, t) = \frac{1}{N}\sum_{j=1}^{N} \delta(v - v_i(z, t)), \qquad f_M^N(z, v, t) = \frac{1}{N}\sum_{j=1}^{N} \delta(v - v_i^M(z, t)).$$

Observe that, for any a test function φ, if we denote by

$$\langle \varphi, f\rangle(z, t) := \int_{\mathbb{R}^d} f(z, v, t)\varphi(v)\, dv,$$

we have

$$\langle \varphi, f^N\rangle(z, t) = \frac{1}{N}\sum_{j=1}^{N} \varphi(v_i(z, t)), \qquad \langle \varphi, f_M^N\rangle(z, t) = \frac{1}{N}\sum_{j=1}^{N} \varphi(v_i^M(z, t)).$$

If we assume that $\int_{\mathbb{R}^d} f(z, v, t)\, dz = 1$, then $\langle \varphi, f\rangle(z, t)$ is the expectation of φ with respect to f, that we will denote as $\mathbb{E}_V[\varphi]$. Similarly, we denote by $\sigma_\varphi^2 = \mathrm{Var}_V(\varphi)$ its variance with respect to f.

For a random variable $V(z,t)$ taking values in $L^2(\Omega)$ we define

$$\|V\|_{L^2(\mathbb{R}^{d_v};L^2(\Omega))} = \mathbb{E}_V\left[\|V\|^2_{L^2(\Omega)}\right]^{1/2}.$$

We have the following result:

Theorem

Let $f(z,v,t)$ a probability density function in v at time $t \geqslant 0$ and $f_M^N(z,v,t)$ the empirical measure of the N-particles sG approximation with M projections associated to the samples $\{v_1(z,t),\dots,v_N(z,t)\}$. Provided that $v_i(z,t) \in H^r(\Omega)$ for all $i = 1,\dots,N$, the following estimate holds

$$\|\langle \varphi, f\rangle - \langle \varphi, f_M^N\rangle\|_{L^2(\mathbb{R}^{d_v};L^2(\Omega))} \leqslant \frac{\|\sigma_\varphi\|_{L^2(\Omega)}}{N^{1/2}} + \frac{C}{M^r}\left(\frac{1}{N}\sum_{i=1}^{N}\|\nabla\varphi(\xi_i)\|_{L^2(\Omega)}\right),$$

where φ is a test function, C is a positive constant independent on M, $\xi_i = (1-\theta)v_i + \theta v_i^M$, $\theta \in (0,1)$.

Numerical examples

Test 1 ($\alpha = 0$): Initial uncertain data

$$f_0(z, v) = \frac{\alpha^2(z)\mathbf{v}^2}{\pi} e^{-\alpha(z)\mathbf{v}^2}, \qquad \mathbf{v} = \sqrt{v_x^2 + v_y^2},$$

so that f_0 has the uncertain temperature

$$T(z) = \frac{1}{\alpha(z)}.$$

An exact solution is given by

$$f(z, v, t) = \frac{1}{2\pi s(z, t)} \left[1 - \frac{1 - \alpha(z) s(z, t)}{\alpha(z) s(z, t)} \left(1 - \frac{\mathbf{v}^2}{2s(z, t)} \right) \right] e^{-\frac{\mathbf{v}^2}{2s(z,t)}},$$

where $s(z, t) = \dfrac{2 - e^{-t/8}}{2\alpha(z)}$.

We will consider

$$\alpha(z) = 2 + \kappa z, \qquad z \sim \mathcal{U}([-1, 1]).$$

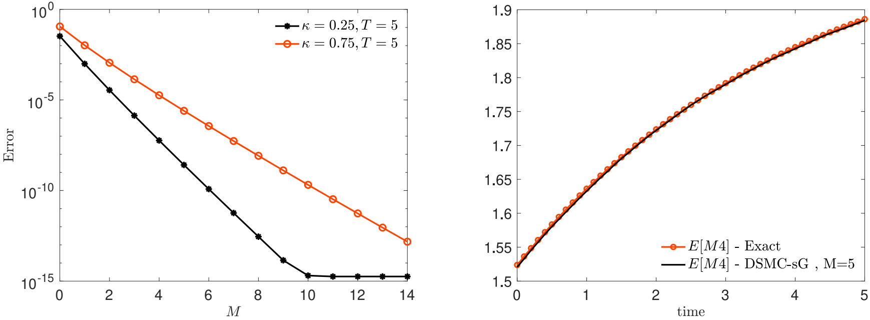


Figure: Left: Convergence of the $L^2(\Omega)$ error with respect to the fourth order moment obtained from a reference solution computed with $N = 10^6$ and $M = 25$ for the DSMC-sG methods. Right: evolution of the fourth order moment in the interval $[0, 5]$ for exact and DSMC-sG approximation with $N = 10^6$ and $M = 5$.

Numerical examples

Test 2 (generic α): Initial data

$$f(z,v,0)=\frac{1}{2\pi\sigma^2(z)}\left[e^{\frac{-|v-2\sigma(z)e_1|^2}{2\sigma^2(z)}}+e^{\frac{-|v+2\sigma(z)e_1|^2}{2\sigma^2(z)}}\right],\quad e_1=(1,0).$$

We check the evolution of the components of the stress tensor

$$P_{ij}(z,t)=\int_{\mathbb{R}^2}(v_i-u_i)(v_j-u_j)f(z,v,t)dv,\qquad i,j=1,2,$$

where u_i are the components of the mean velocity.

For $\alpha=0$, we have an exact evolution of the components of the stress tensor

$$P_{11}(z,t)=T(z)+\frac{1}{2}w(t),\qquad P_{22}(z,t)=T(z)-\frac{1}{2}w(t),$$

being $T(z)=\sigma^2(z)$ the temperature, $w(t)=w_0e^{-t/2}$ and $w_0=4\pi$.

We will consider

$$\sigma(z)=\frac{\lambda}{6}\left(1+\kappa z\right),\qquad z\sim\mathcal{U}([-1,1]),\quad \lambda=\frac{2\pi}{3+\sqrt{2}}.$$

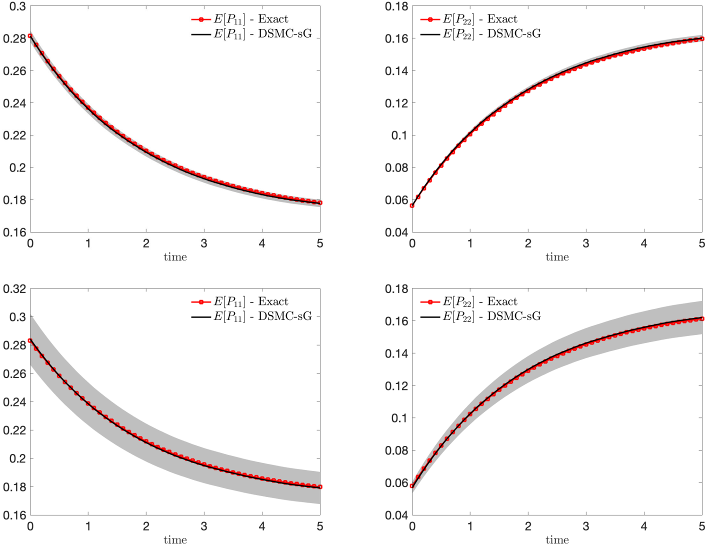


Figure: Evolution of the expected $P_{11}(z,t)$ and $P_{22}(z,t)$ in the case $\alpha = 0$ and two level of uncertainty $\kappa = 0.1$ (top) and $\kappa = 0.5$ (bottom). We compare the exact evolution with the DSMC-sG scheme with $N = 10^6$ particles and $M = 5$ Galerkin projections.

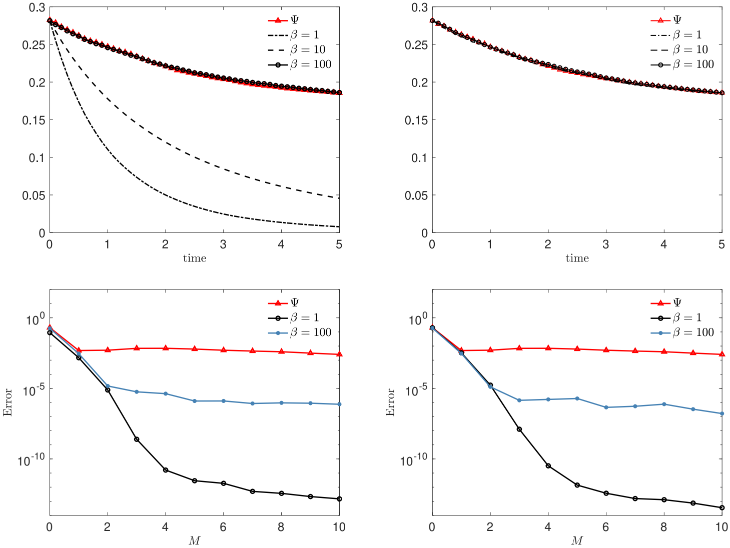


Figure: Expectation of $P_{11}(z, t)$ in time for $\alpha = 1$ (top) and L^2 error of the DSMC-sG scheme at $t = 1$ with respect to M (bottom). The indicator function $\Psi(\cdot)$ has been regularized as $(\tanh(\beta(\cdot)) + 1)/2$ (left) and imposing energy conservation (right).

Conclusions

- We introduced a novel hybrid approach for uncertainty quantification in collisional kinetic equations of Boltzmann type.
- The method combines an efficient DSMC solver in the physical space with a stochastic Galerkin method in the random space.
- The coupling amounts on a gPC expansion of the statistical samples and on the Galerkin projection of the corresponding DSMC solver.
- In particular, in the variable hard sphere case, this requires a suitable reformulation of the classical DSMC method.
- The methodology here presented is fully general and can be extended to other Boltzmann-type equations outside the classical rarefied gas dynamics setting.
- Convergence results for space homogeneous problems.
- Extension of the methods to the Landau-Fokker-Planck equation of plasma physics and applications to space non homogenous problems.

More details:

L. Pareschi, M.Zanella, arXiv:2003.06716, (2020)