Stochastic Galerkin particle methods for kinetic equations of plasmas with uncertain data

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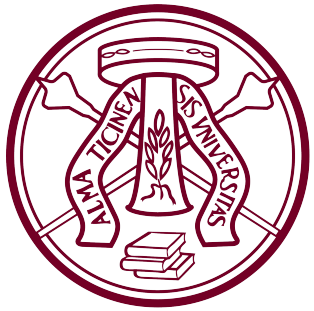
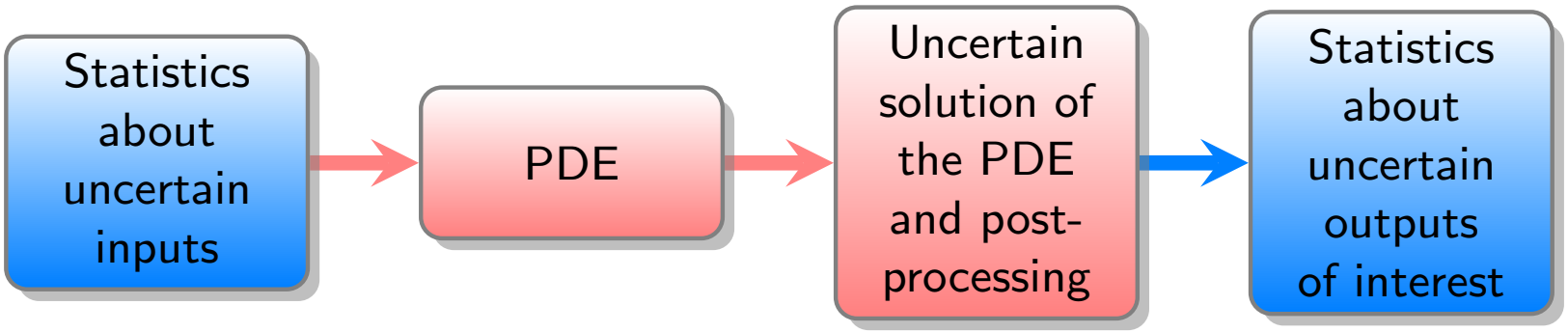


Webinar Kinetic and fluid equations for collective behavior

Joint Work with Andrea Medaglia (Unipv), Lorenzo Pareschi (Unife)

Outline

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 the propagation of missing information with respect to some quantity of interest (a quantity that depends on the solution of the PDE).
- 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 quantification

- Monte Carlo method is non-intrusive with low computational cost and easy to parallelize, it does not require knowledge of PDF or regularity in the random space. The convergence of such methods is slow.
- Stochastic Galerkin (sG) methods are intrusive methods based on *suitable projections* in polynomial spaces of the original problem[1]. Such methods are spectrally accurate provided propagation of regularity. They suffer the curse of dimensionality, the main properties of the solution, like positivity, are lost.
- Multifidelity methods based on the use of control variate techniques[2]. These methods are more efficient than Galerkin's stochastic approaches for problems with high dimensionality of the random 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,Q.Li,L.Liu,R.Shu,Y.Zhu, ..., '16-'22; L.Pareschi et al. '18-'22: B.Despres '10
[2] G.Dimarco, L.Pareschi '19-'20; L.Liu, X.Zhu '20; L. Pareschi, J. Hu, Y. Wang '21
[3] J.A.Carrillo, A.Medaglia, L.Pareschi, M.Z. '18-'23

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Uncertainties in homogeneous kinetic equations

Let us focus on the case of the homogeneous Boltzmann equation

$$\partial_t f(\mathbf{z}, x, v, t) + v \cdot \nabla_x f(\mathbf{z}, x, v, t) = \frac{1}{\varepsilon(\mathbf{z})} Q(f, f)(\mathbf{z}, x, v, t), \qquad x, v \in \mathbb{R}^{d_v}, t \geq 0$$

with $\varepsilon > 0$ the Knudsen number and $\mathbf{z} \in I_{\mathbf{z}} \subseteq \mathbb{R}^{d_z}$ a random vector $\sim p(\mathbf{z})$. The *Boltzmann collision operator* has the form

$$Q(f, f)(\mathbf{z}, x, v, t) = \int_{\mathbb{S}^{d_v - 1} \times \mathbb{R}^{d_v}} B\left(|q|, \frac{q \cdot n}{|q|}\right) \left(f(v') f(v'_*)_* - f(v) f(v_*)\right) dn \, dv_*.$$

where $q = v - v_*$ and the binary interaction rules are given by

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

The kernel $B(|q|, \cos\theta) \geq 0$ reads

$$B(|q|, \cos\theta) = |q| \sigma(|q|, \theta), \qquad 0 \leq \theta \leq \pi, \cos\theta = \frac{q \cdot n}{|q|},$$

here $\sigma(|q|, \theta)$ is the differential cross section at scattering angle θ.

Collision kernel

We define the total scattering and the momentum-transfer cross section respectively as follows

$$\sigma_{tot}(|q|) = 2\pi \int_0^\pi \sigma(|q|,\theta)\sin\theta d\theta, \quad \sigma_{tr}(|q|) = 2\pi \int_0^\pi \sigma(|q|,\theta)(1-\cos\theta)\sin\theta d\theta.$$

Amongst the relevant cases we mention the VHS model for which

$$\sigma(|q|,\theta) = C_\gamma |q|^{\gamma-1} \Rightarrow B(|q|,\theta) = C_\gamma |q|^\gamma,$$

and therefore $\sigma_{tot} = \sigma_{tr} = 4\pi C_\gamma |q|^{\gamma-1}$. Whereas, if particles are subject to Coulomb forces, according to the Rutherford formula, we should consider

$$\sigma(|q|,\theta) = \frac{b_0^2}{4\sin^4(\theta/2)}, \qquad b_0 = \frac{e^2}{4\pi\epsilon_0 m_r |q|^2},$$

which become singular for $\theta \to 0$ and we have $\sigma_{tot} = \pi\lambda_d^2$, $\sigma_{tr} = 4\pi b_0^2 \log\Lambda$ where $\Lambda = \sin^{-1}(\theta^{min}/2)$.

Reformulation of DSMC for VHS with uncertainty

We consider first the VHS case. Denote by $Q_\Sigma(f,f)$ the collision operator with the kernel

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

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

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

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

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

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

Stochastic Galerkin approximation

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

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

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

$$\int_{\mathbb{R}^{d_z}} \Psi_n(\mathbf{z}) \Psi_m(\mathbf{z}) p(\mathbf{z}) \, d\mathbf{z} = \mathbb{E}_{\mathbf{z}}[\Psi_m(\cdot)\Psi_n(\cdot)] = \delta_{mn}, \qquad m, n = 0, \dots, M,$$

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

$$\hat{v}_{i,m}(t) = \int_{\mathbb{R}^{d_z}} v_i(\mathbf{z}, t) \Psi_m(\mathbf{z}) p(\mathbf{z}) \, d\mathbf{z} = \mathbb{E}_{\mathbf{z}}[v_i(\cdot, t)\Psi_m(\cdot)].$$

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

Stochastic Galerkin approximation

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

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

where

$$\begin{aligned} \hat{W}^m_{ij}(\xi, t) &= \int_{\mathbb{R}^{d_z}} \chi(\Sigma\,\xi < B_{ij}(\mathbf{z}))\left(v^M_i(\mathbf{z}, t) - v^M_j(\mathbf{z}, t)\right)\Psi_m(\mathbf{z})p(\mathbf{z})\, d\mathbf{z}, \\ \hat{V}^m_{ij}(\xi, t) &= \int_{\mathbb{R}^{d_z}} \chi(\Sigma\,\xi < B_{ij}(\mathbf{z}))|v^M_i(\mathbf{z}, t) - v^M_j(\mathbf{z}, t)|\Psi_m(\mathbf{z})p(\mathbf{z})\, d\mathbf{z}. \end{aligned}$$

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 $O(MH)$.

Consistency estimate on moments

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

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

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

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

we have

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

If we assume that $\int_{\mathbb{R}^d} f(\mathbf{z}, v, t)\, dv = 1$, then $\langle \varphi, f \rangle(\mathbf{z}, t)$ 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.

Consistency estimate on the moments

For a random variable $V(\mathbf{z},t)$ taking values in $L^2(\mathbb{R}^{d_z})$ we define

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

We have the following result:

Theorem (L. Pareschi, M.Z. '20)

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

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

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

VHS model: 2D Maxwellian case ($\gamma = 0$)

Initial uncertain data

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

so that f_0 has the uncertain temperature

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

An *exact solution* is given by

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

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

We will consider

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

VHS model: 2D Maxwellian case ($\gamma = 0$)

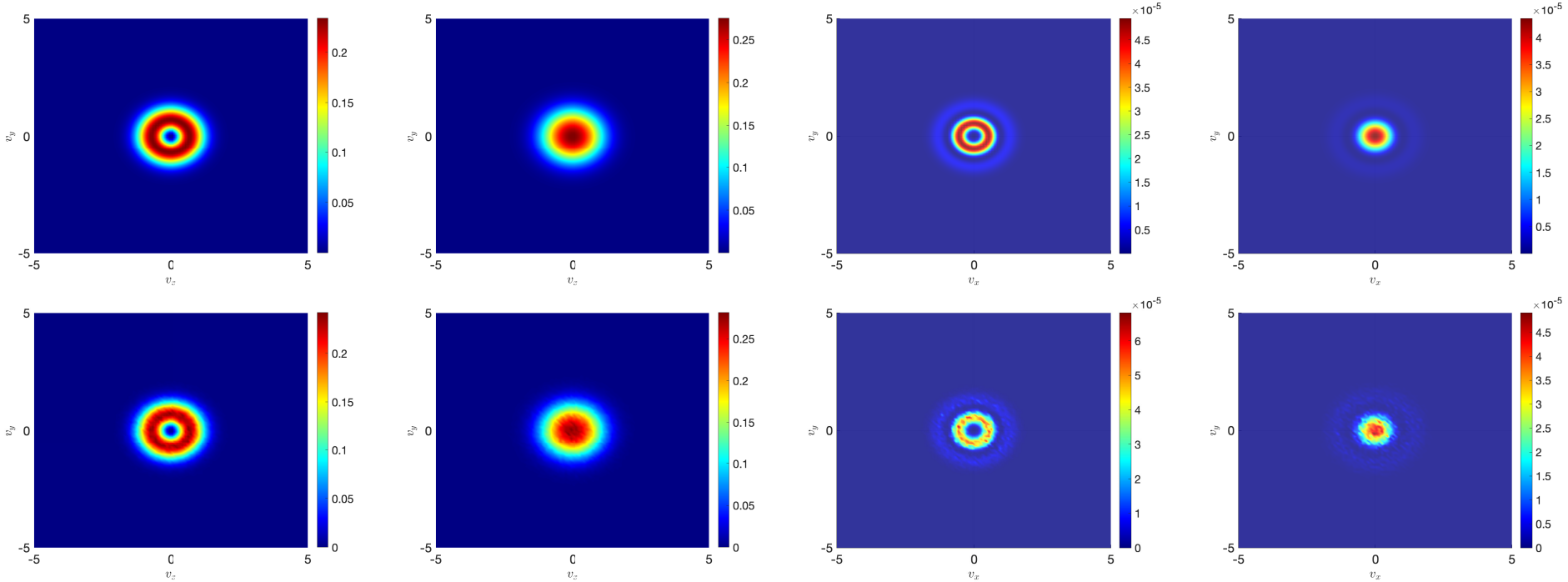


Figure: Expected distribution $\mathbb{E}[f]$ and variance $\mathrm{Var}(f)$ of the 2D Boltzmann model for Maxwell molecules for exact (top tow) and DSMC-sG approximation (bottom row) with $N = 10^6$ and $M = 5$.

VHS model: 2D Maxwellian case ($\gamma = 0$)

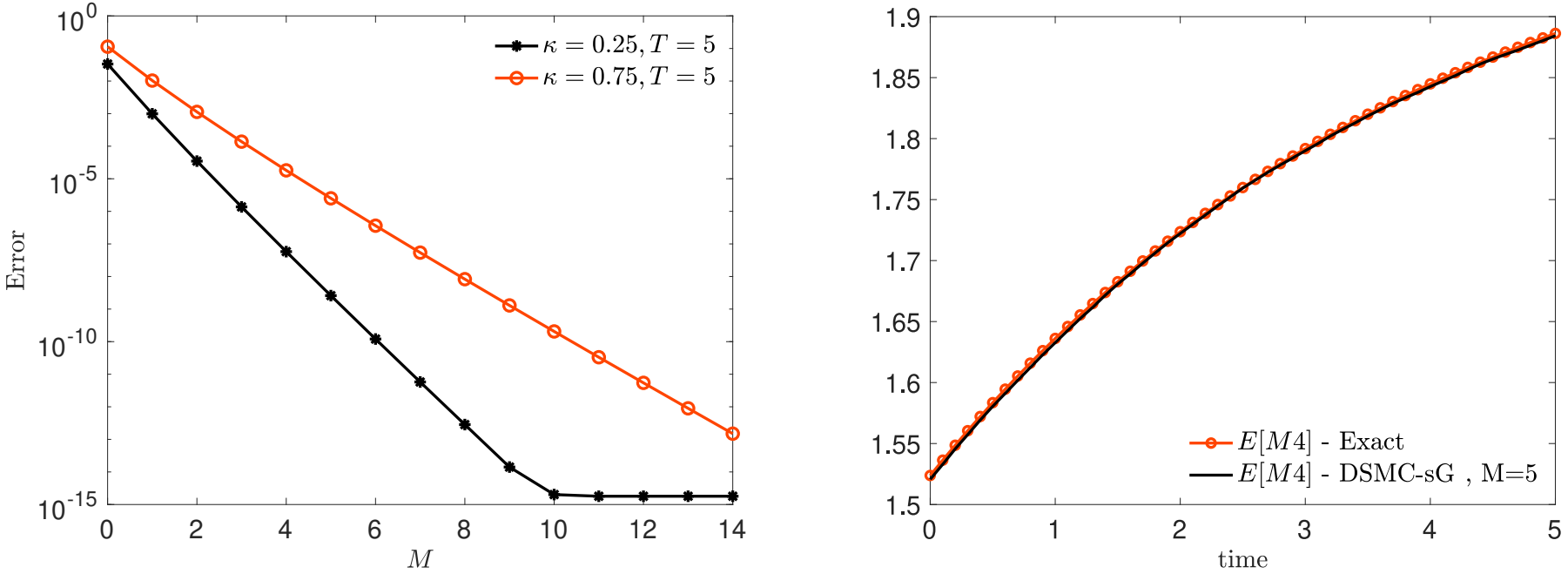
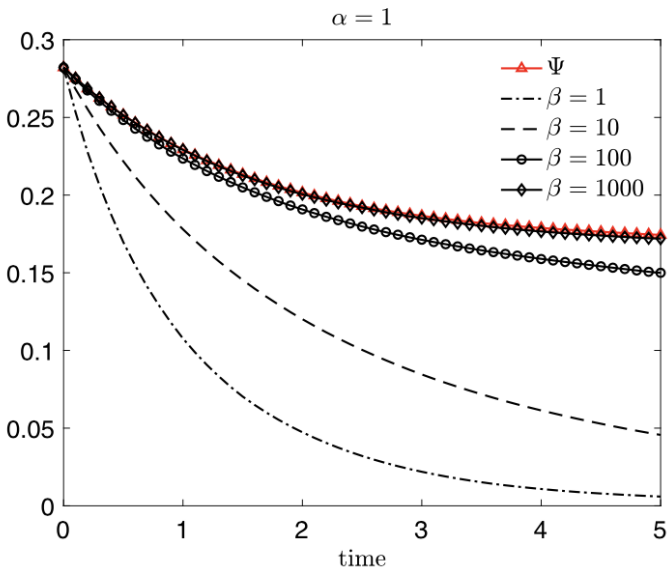
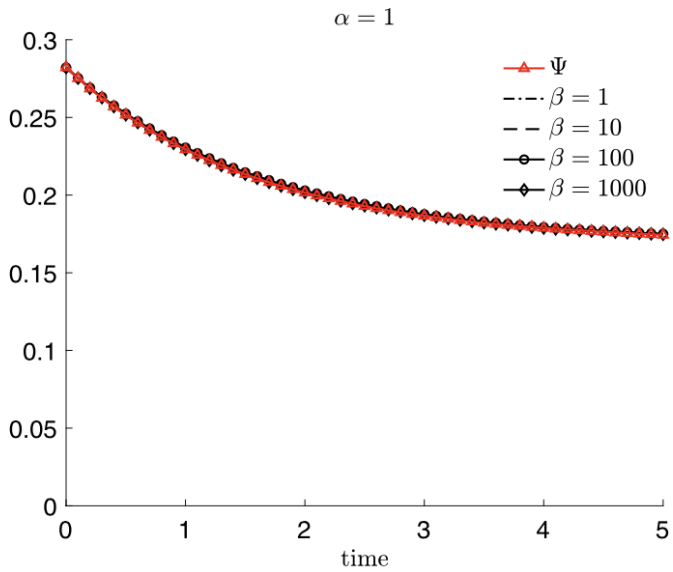
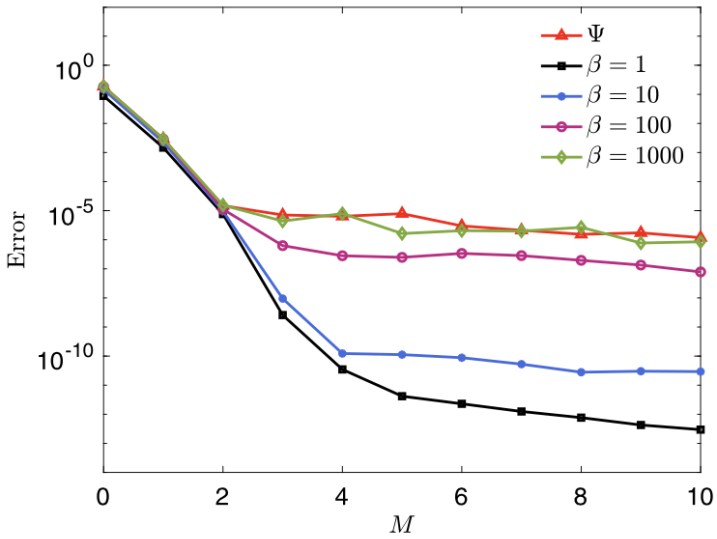


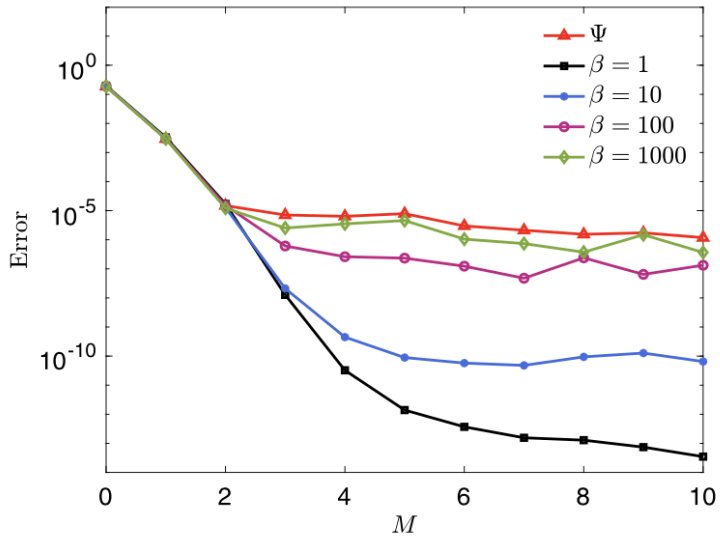
Figure: Left: Convergence of the $L^2(\Omega)$ error with respect to the fourth order moment obtained from a reference solution computed with $N = 10^6$ and $M = 25$ for the DSMC-sG methods. Right: evolution of the fourth order moment in the interval $[0, 5]$ for exact and DSMC-sG approximation with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

Numerical examples: VHS case ($\gamma = 1$)









The Landau-Fokker-Planck equation

Let us consider the Landau collision operator

$$Q(f,f)(\mathbf{z},v,t) = \nabla_v \cdot \int_{\mathbb{R}^3} \Phi(q)\left[f(\mathbf{z},v_*)\nabla_v f(\mathbf{z},v) - f(\mathbf{z},v)\nabla_{v_*} f(\mathbf{z},v_*)\right] dv_*,$$

where Φ is a 3×3 nonnegative symmetric matrix defining the interactions between particles

$$\Phi(q) = |q|^{\gamma+2} S(q), \qquad S(q) = I - \frac{q\otimes q}{|q|^2},$$

where $\gamma = -3$ gives the so-called Coulomb case. The large time behaviour of undertain Landau equation is the Maxwellian distribution

$$\mathcal{M}(\mathbf{z},v) = \left(\frac{1}{2\pi T(\mathbf{z})}\right)^{3/2} \exp\left(-\frac{v-U(\mathbf{z})^2}{2T(\mathbf{z})}\right),$$

where $U(\mathbf{z})$ and $T(\mathbf{z})$ are the uncertain momentum and kinetic temperature of the system.

Numerical methods in plasma physics: brief overview

The numerical methods for plasma physics developed in the literature can be essentially divided into two groups:

1. approaches based on direct discretizations of the corresponding system of partial differential equations (PDEs), like finite differences/volumes methods [4] and semi-Lagrangian schemes [5] or Fourier spectral methods [6],
2. approaches based on approximations of the underlying particle dynamics at different levels, like particle-in-cell (PIC) methods [7], direct simulation Monte Carlo (DSMC) methods for kinetic equations [8], deterministic particle methods.[9]

[4] N.Crouseilles, F.Filbet '04; F.Filbet, E.Sonnendrücker, P.Bertrand '01; G.Dimarco, Q.Li, L.Pareschi, B.Yan '15;

[5] E. Sonnenrücker; J.Roche, P.Bertrand, A.Ghizzo '99

[6] I.Gamba, J.Haack, C.Hauck, J.Hu '17; J.Hu, S.Jin '16; L.Pareschi, G.Russo, G.Toscani '00

[7] C.K. Birdsall, A.B. Langdon '85; E.Sonnendrücker and coworkers

[8] A.V.Bobylev, K.Nanbu '00; R.Caflish, C. Wang, G.Dimarco, B.Cohen, A.Dimits '08; L.F.Ricketson, M.S.Rosin, R.Caflisch, A.M.Dimits '14

[9] J.A.Carrillo, J.Hu, L.Wang, J.Wu '20; J.A. Carrillo, S.Jin, Y.Tang '22

First order approximation of the Boltzmann operator

It is well-known that in the grazing collision limit we can recover the Landau-Fokker-Planck equation from a Boltzmann operator with collision kernel with Coloumb forces. [10] We get the first order approximation

$$\partial_t f(v,t) = \frac{1}{\epsilon}\left[\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} D(\mu,\tau_0) f(v') f(v'_*)\, dn\, dv_* - \rho f(v)\right],$$

where $\mu = \omega \cdot n$, $\omega = q/|q|$ and

$$D(\mu,\tau_0) = \sum_{\ell=0}^{+\infty} \frac{2\ell+1}{4\pi} P_\ell \exp\left\{-\ell(\ell+1)\tau_0\right\}, \qquad \tau_0 = \frac{\epsilon}{2}|q|\sigma_{tr}(|q|).$$

Simpler collision kernels $D_*(\mu,\tau_0)$ should satisfy

1. $D_*(\mu,\tau_0) \geq 0$ and $2\pi \int_{-1}^{1} D_*(\mu,\tau_0) d\mu = 1$
2. $\lim_{\tau_0 \to 0} D_*(\mu,\tau_0) = \frac{1}{2\pi}\delta(1-\mu)$
3. $\lim_{\tau \to 0} \frac{2\pi}{\tau_0} \int_{-1}^{1} (D_*(\mu,\tau_0) - D(\mu,\tau_0)) P_\ell(\mu) = 0$

[10] A.V.Bobylev, K.Nanbu '00

Approximated collision kernels

Lemma (Bobylev-Nanbu '00)

The conditions 1-2-3 are satisfied by any function

$$D_*(\mu,\tau_0)=\psi\left(\frac{1-\mu}{2\tau_0}\right)\left(4\pi\tau_0\int_0^{1/\tau_0}\psi(x)dx\right)^{-1}$$

with $\psi(x)\geq 0$ *for* $x>0$ *and*

- $\int_0^{+\infty}\psi(x)dx=\int_0^{+\infty}x\psi(x)dx<+\infty$
- $\lim_{\tau_0\to 0}\int_{1/\tau_0}^{+\infty}x^n\psi(x)dx=0$, *for any* $n=2,3,\dots$.

We compare 3 different approximated kernels

$i)$ It has been considered[11]

$$D_*^{(1)}(\mu,\tau_0)=\frac{A}{4\pi\sinh A}\exp\{\mu A\},$$

with $\coth A-A^{-1}=\exp\{-2\tau_0\}$.

[11] K.Nanbu '97; R. Caflisch, G. Dimarco, L.Pareschi '10

Approximated collision kernels

which leads to spherical coordinates (θ, ϕ) defined as

$$\cos\theta = \frac{1}{A}\log\left(\exp\{-A\} + 2r_1 \sinh A\right)$$
$$\phi = 2\pi r_2, \qquad r_1, r_2 \sim \mathcal{U}([0,1])$$

ii) A simplification has been provided in [A.V. Bobylev, K.Nanbu '00] and is

$$D_*^{(2)}(\mu, \tau_0) = \frac{1}{2\pi}\delta(\mu - \nu(\tau_0)), \quad \nu(\tau_0) = \begin{cases} 1 - 2\tau_0 & 0 \le \tau_0 \le 1 \\ -1 & \tau_0 > 1 \end{cases}$$

Sampling from $D_*^{(2)}(\mu, \tau_0)$ corresponds in the spherical coordinates to fix θ as $\cos\theta = \nu(\tau_0)$ and compute $\phi = 2\pi r_2$, $r_2 \sim \mathcal{U}([0,1])$.

iii) A third approximation[12] is given by

$$D_*^{(3)}(\mu, \tau_0) = \frac{1}{2\pi}\delta(\mu - \tilde{\nu}(\tau_0)), \quad \tilde{\nu}(\tau_0) = 1 - 2\tanh\tau_0.$$

Sampling from $D_*^{(3)}(\mu, \tau_0)$ corresponds in the spherical coordinates to compute (θ, ϕ) as follows

$$\cos\theta = \tilde{\nu}(\tau_0), \qquad \phi = 2\pi r_2$$

[12] A.Medaglia,L.Pareschi, M.Z. '23

Nanbu 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[13].

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

$$f^{n+1} = \left(1 - \frac{\Delta t}{\epsilon}\right) f^n + \frac{\Delta t}{\epsilon} P^{(i)}_{*,\epsilon}(f^n, f^n),$$

where

$$P^{(i)}_{*,\epsilon}(f, f) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} D^{(i)}_*(\mu, \tau_0) f(v') f(v'_*)\, dv_*\, dn,$$

where we substituted $D(\mu, \tau_0)$ by any of the previous approximations $D^{(i)}_*$, $i = 1, 2, 3$ previously defined. If f^n is a probability density then both $P_{*,\epsilon}$ and f^{n+1} are probability densities provided $\Delta t \leq 1$.

[13] K. Nanbu '83, H. Babovski '86

Nambu DSMC scheme

Hence, the collision law of two colliding particles reads

$$v_i' = v_i^n - \frac{1}{2}\left(q^n(1-\cos\theta) + h^n \sin\theta\right)$$
$$v_j' = v_j^n + \frac{1}{2}\left(q^n(1-\cos\theta) + h^n \sin\theta\right)$$

where $q^n = v_i^n - v_j^n$ and

$$h_x^n = q_\perp^n \cos\phi$$
$$h_y^n = -(q_y^n q_x^n \cos\phi + q^n q_z^n \sin\phi)/q_\perp^n$$
$$h_z^n = -(q_z^n q_x^n \cos\phi - q^n q_y^n \sin\phi)/q_\perp^n,$$

with $q_\perp^n = \sqrt{(q_y^n)^2 + (q_z^n)^2}$

Reformulation of DSMC with uncertainties

Given the PDF $p(\mathbf{z})$ a pair of colliding particles is approximated as

$$v_\ell^{n,M} = \sum_{k=0}^{M} \hat{v}_{\ell,k}^n \Psi_k(\mathbf{z}), \qquad \hat{v}_{\ell,k}^n = \mathbb{E}_{\mathbf{z}}[v_\ell^n(\mathbf{z})\Psi_k(\mathbf{z})], \quad \ell \in \{i,j\}$$

$$q_{ij}^{n,M} = \sum_{k=0}^{M} \hat{q}_{ij}^n \Psi_k(\mathbf{z}), \qquad \hat{q}_{ij,k}^n = \hat{v}_{i,k}^n - \hat{v}_{j,k}^n$$

Therefore, if we recall that $\tau_0 = \tau_0(\mathbf{z})$ and $\theta = \theta_{ij}(\mathbf{z})$ we obtain the following interaction scheme for each projection $k = 0, \dots, M$

$$\hat{v}'_{i,k} = \hat{v}_{i,k}^n - \frac{1}{2}\left(\hat{q}_{ij,k}^n - \sum_{\ell=0}^{M} \hat{q}_{ij,\ell}^n \hat{V}_{\ell k}^n + \hat{W}_k^n\right)$$

$$\hat{v}'_{j,k} = \hat{v}_{j,k}^n + \frac{1}{2}\left(\hat{q}_{ij,k}^n - \sum_{\ell=0}^{M} \hat{q}_{ij,\ell}^n \hat{V}_{\ell k}^n + \hat{W}_k^n\right),$$

where

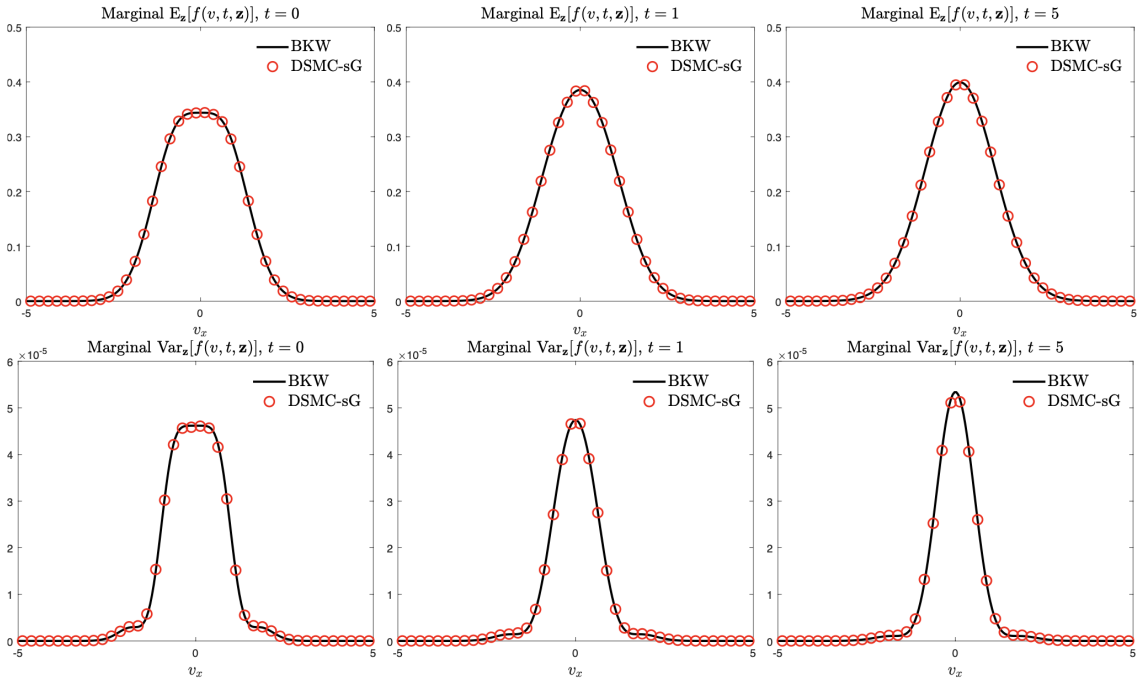
$$\hat{V}_{\ell k}^n = \int_{I_{\mathbf{z}}} \cos\theta_{ij}(\mathbf{z})\Psi_\ell(\mathbf{z})\Psi_k(\mathbf{z})p(\mathbf{z})d\mathbf{z}, \;\; \hat{W}_{ij,k}^n = \int_{I_{\mathbf{z}}} h_{ij,k}^{n,M}(\mathbf{z}) \sin\theta_{ij}(\mathbf{z})\Psi_k(\mathbf{z})p(\mathbf{z})d\mathbf{z}.$$

BKW solution with uncertainties

We consider the model with Maxwell molecules and uncertain initial temperature

$$f(\mathbf{z}, v, t) = \frac{1}{2\pi K(\mathbf{z}, t)} e^{-\frac{|v|^2}{2K(\mathbf{z},t)}} \left(\frac{5K(\mathbf{z}, t) - 3T(\mathbf{z})}{2K(\mathbf{z}, t)} + \frac{T(\mathbf{z}) - K(\mathbf{z}, t)}{2K(\mathbf{z}, t)} |v|^2 \right),$$

with $K(\mathbf{z}, t) = T(\mathbf{z}) \left(1 - \frac{2}{5} e^{t/2}\right)$, $T(\mathbf{z}) = \kappa + 0.1\mathbf{z}$ and $\mathbf{z} \sim \mathcal{U}([0, 1])$.



Click for video

Coulomb case with uncertainties

We consider $T(\mathbf{z}) = \frac{1}{3}(T_x(\mathbf{z},t) + T_y(\mathbf{z},t) + T_z(\mathbf{z},t))$ with uncertain initial conditions in the temperature along the x-axis: $T_x(\mathbf{z},0) = 1 + 0.05\mathbf{z}$, $T_y(0) = 0.75$, $T_z(0) = 0.5$ and $\mathbf{z} \sim \mathcal{U}([0,1])$.

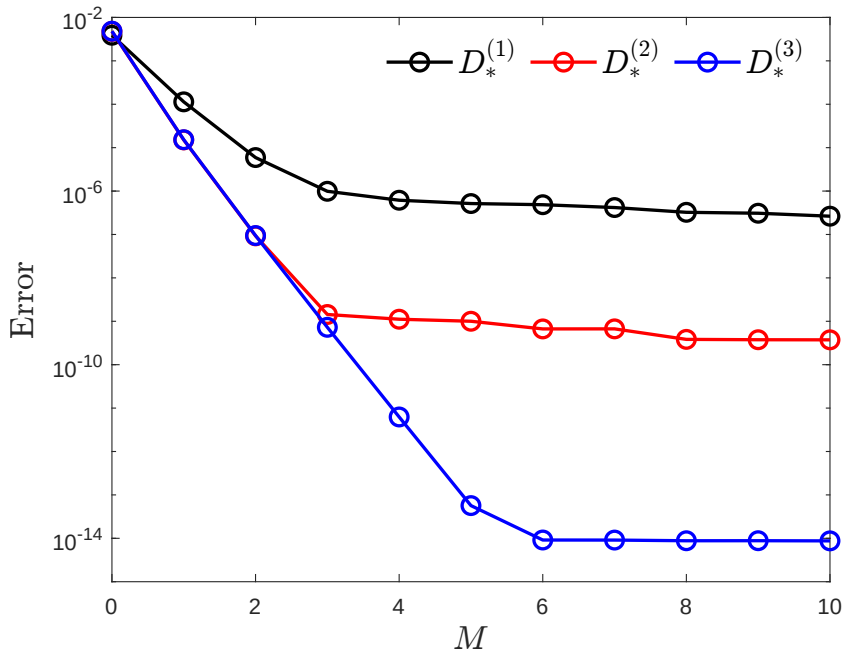


Figure: L^2 error of the temperature $T(\mathbf{z})$ for different kernels, for increasing M, with the NB scheme. We choose $N = 10^6$, $\Delta t = \epsilon = 0.1$ and the reference solution is computed with an order $M = 30$.

Trubnikov test

We define the initial distribution

$$f_0(\mathbf{z}, v) = \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{T_x(\mathbf{z},0)T_y(\mathbf{z},0)T_z(\mathbf{z},0)}} e^{-\frac{v_x^2}{2T_x(\mathbf{z},0)}} e^{-\frac{v_y^2}{2T_y(\mathbf{z},0)}} e^{-\frac{v_z^2}{2T_z(\mathbf{z},0)}}.$$

with $T_x(\mathbf{z},0) = T_y(\mathbf{z},0) = 0.08 + 0.04\mathbf{z} > T_z(\mathbf{z},0) = 0.04$. In the case of small uncertain temperature difference the Trubnikov solution is

$$\Delta T(\mathbf{z},t) = T_\perp(\mathbf{z},t) - T_z(\mathbf{z},t) = \Delta T(\mathbf{z},0)\exp\{-t/\tau_T\},$$

with $\tau_T = \frac{5}{8}\sqrt{2\pi}\left(\frac{8\sqrt{m}}{\pi\sqrt{2}}\frac{T(\mathbf{z})^{3/2}}{e^4\rho\log\Lambda}\right)$

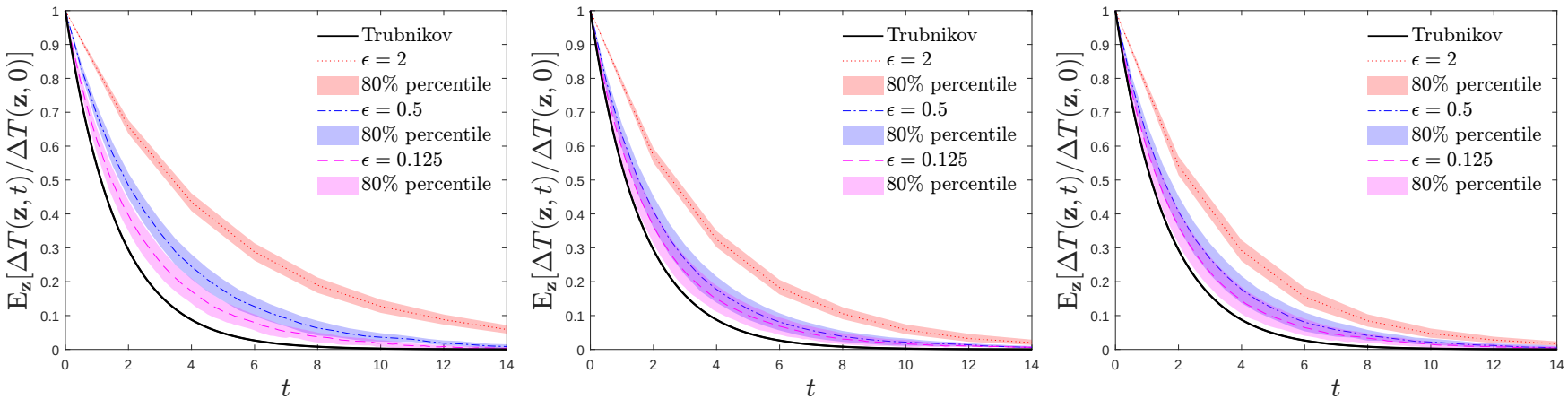
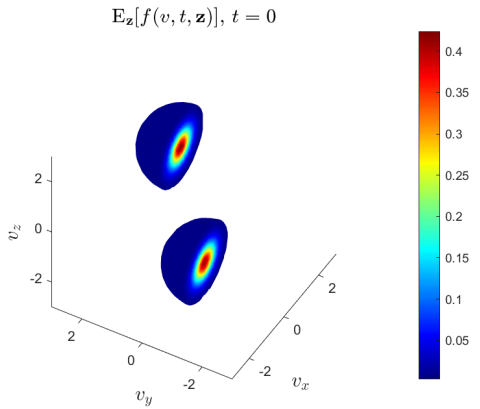
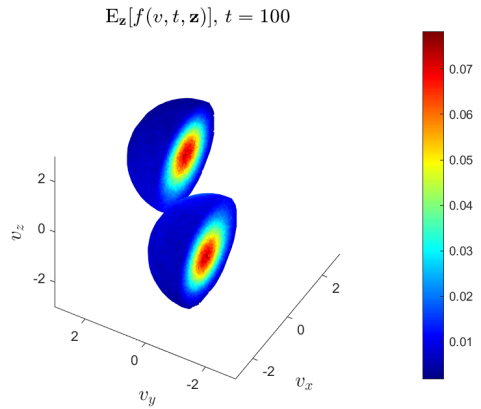
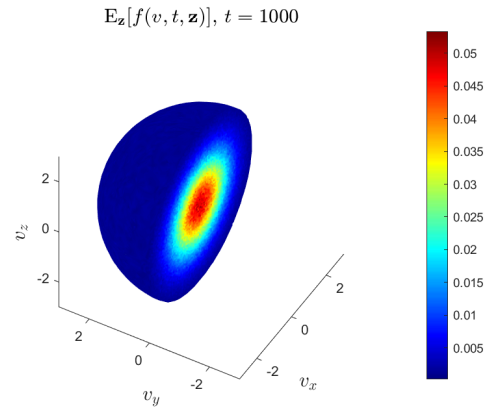


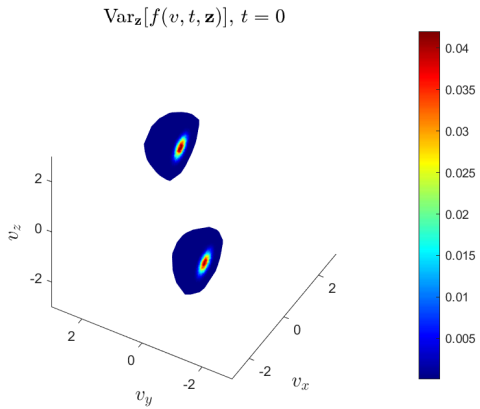
Figure: Time evolution of the expectation of $\Delta T(\mathbf{z},t)/\Delta T(\mathbf{z},0)$, for different values of the scale parameter ϵ, for $D_*^{(1)}$ (left), $D_*^{(2)}$ (centre), and $D_*^{(3)}$ (right).

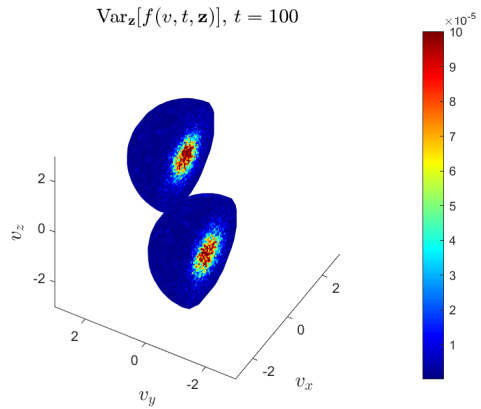
Sum of two Gaussians

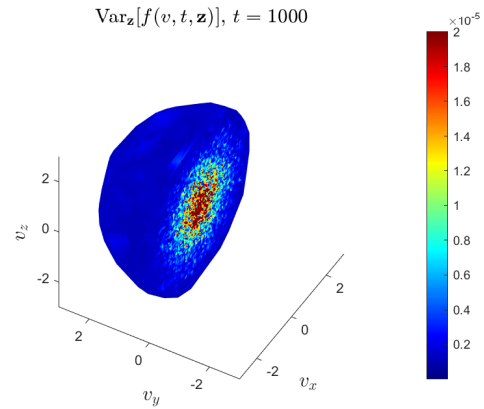


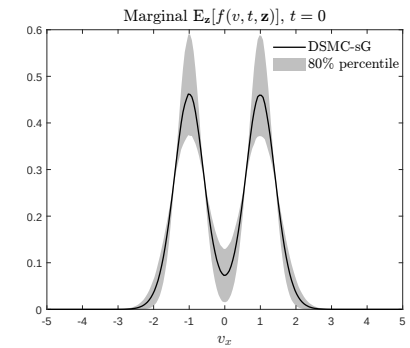


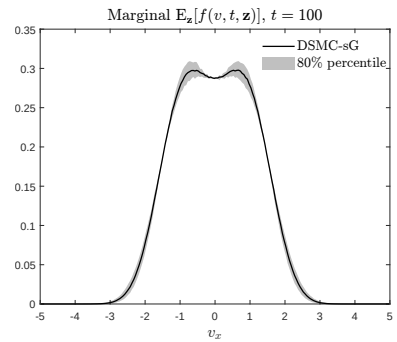


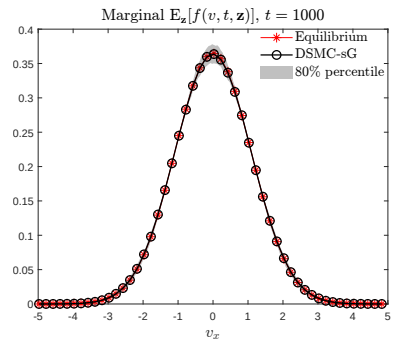




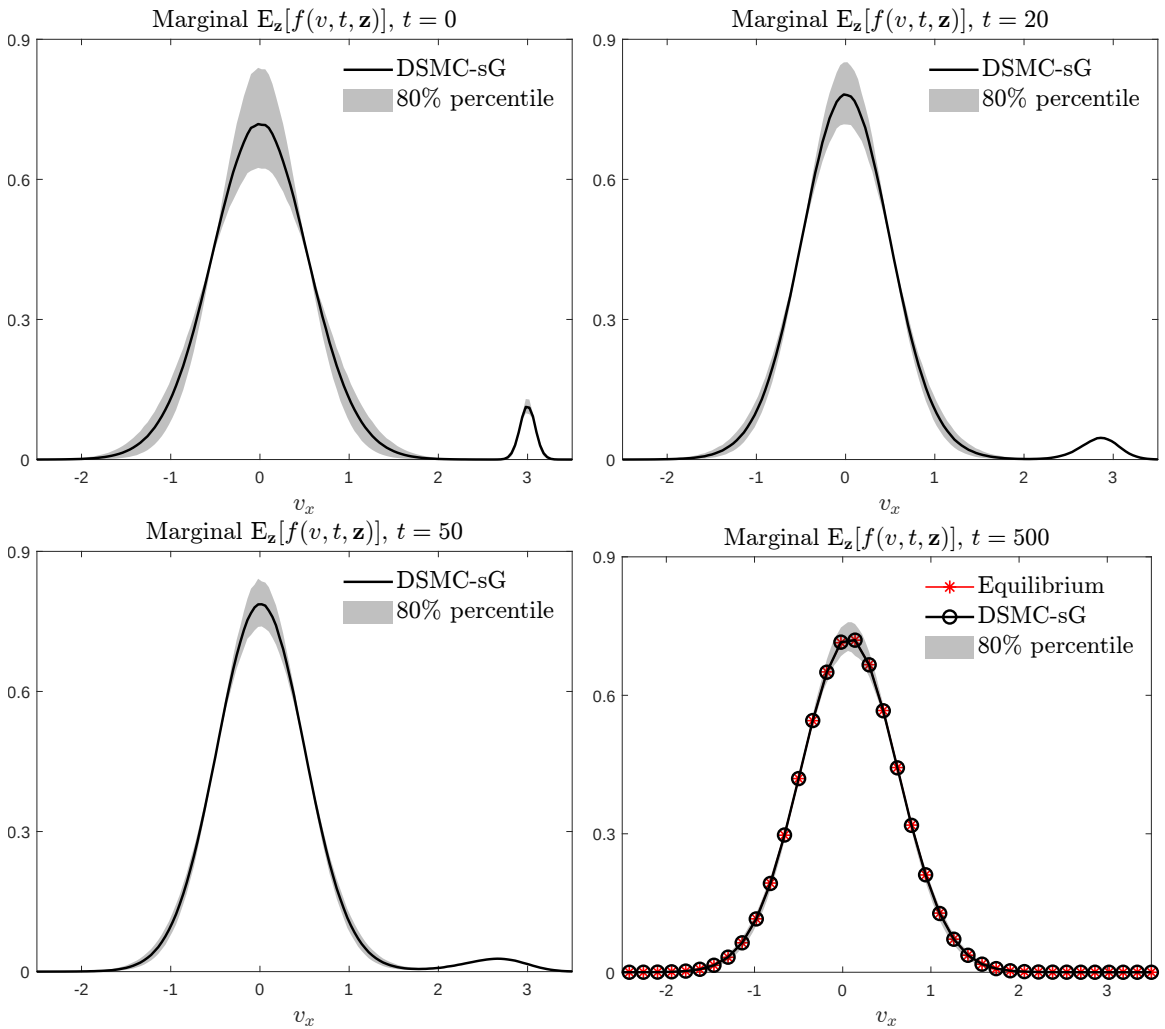








Bump on tail

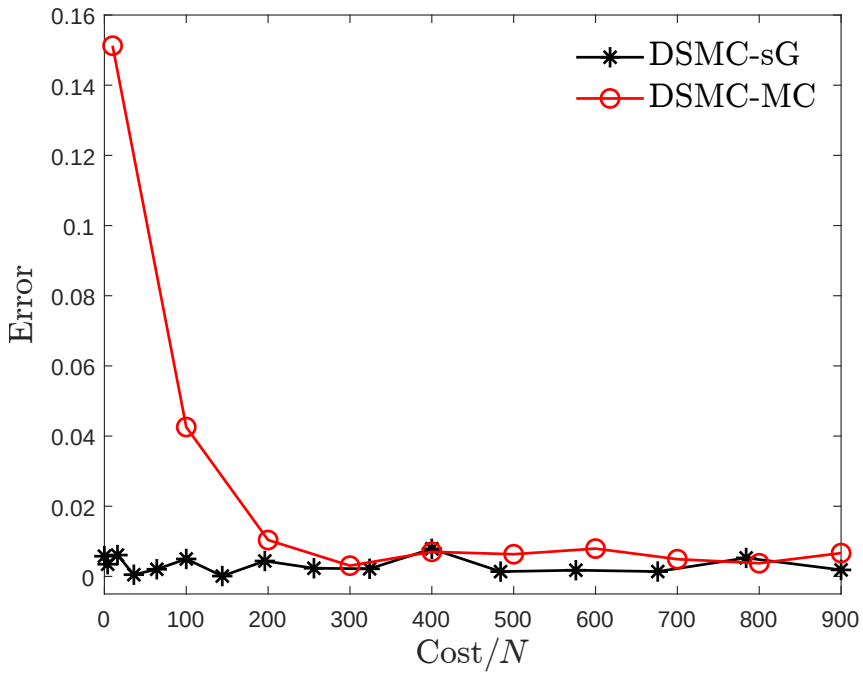

Marginal $\mathrm{E}_{\mathbf{z}}[f(v,t,\mathbf{z})]$, $t = 0$
DSMC-sG
80% percentile
v_x
Marginal $\mathrm{E}_{\mathbf{z}}[f(v,t,\mathbf{z})]$, $t = 20$
DSMC-sG
80% percentile
v_x
Marginal $\mathrm{E}_{\mathbf{z}}[f(v,t,\mathbf{z})]$, $t = 50$
DSMC-sG
80% percentile
v_x
Marginal $\mathrm{E}_{\mathbf{z}}[f(v,t,\mathbf{z})]$, $t = 500$
Equilibrium
DSMC-sG
80% percentile
v_x

DSMC-sG versus DSMC-MC

We fix the number of particles $N = 10^6$, the time step $\Delta t = \epsilon = 0.1$, and we compute the error in the evaluation of the fourth order moment at fixed time $t = 1$

$$\text{Error} = |\mathbb{E}_{\mathbf{z}}[M4(\mathbf{z}, t)] - \mathbb{E}_{\mathbf{z}}[\tilde{M}4(\mathbf{z}, t)]|,$$

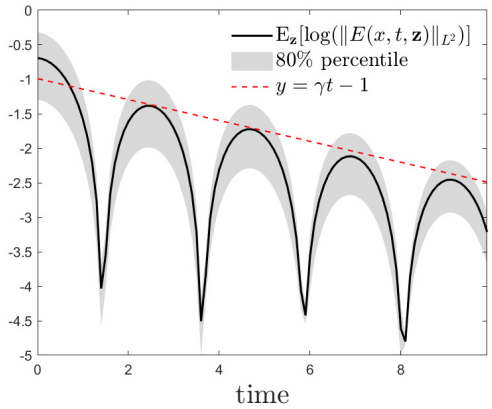
We compare the error with the computational cost that is $O(NM^2)$ for the DSMC-sG scheme and $O(NM)$ for a DSMC-MC scheme.

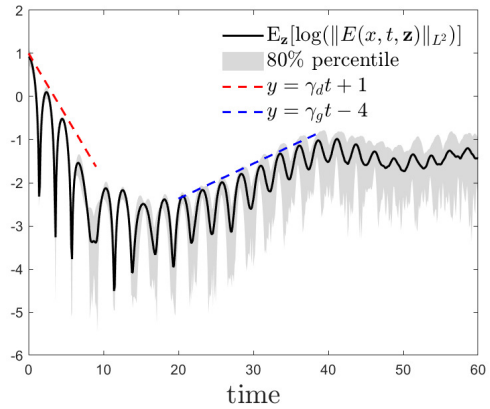


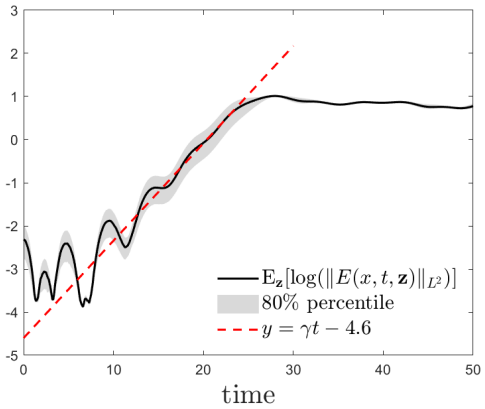
Non-homogeneous problems

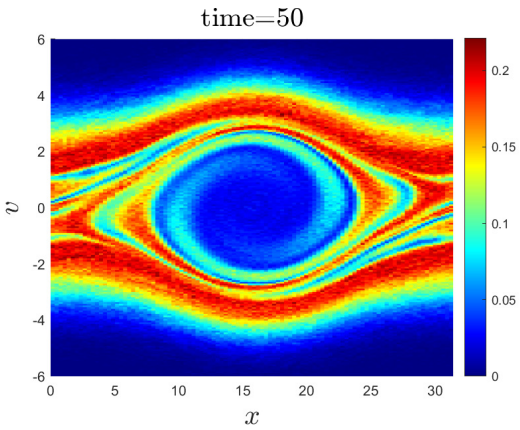
$$\partial_t f(\mathbf{z}, x, v, t) + v \cdot \nabla_x f(\mathbf{z}, x, v, t) + E(\mathbf{z}, x, t) \cdot \nabla_v f(\mathbf{z}, x, v, t) = \frac{1}{\epsilon} Q(f, f)(\mathbf{z}, x, v, t),$$

$$E(\mathbf{z}, x, t) = -\nabla_x \phi(\mathbf{z}, x, t), \quad \Delta_x \phi(\mathbf{z}, x, t) = 1 - \int_{\mathbb{R}^3} f(\mathbf{z}, x, v, t) dv,$$









Euler-Poisson equation with uncertainties

In the limit $\epsilon \to 0$ we obtain $f(\mathbf{z}, x, v, t) = \mathcal{M}_{\rho,U,T}(\mathbf{z}, x, v)$ and, thus, we recover the Euler-Poisson system

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot (\rho U) &= 0 \\ \partial_t (\rho U) + \nabla_x \cdot (\rho U \otimes U) + \nabla_x p &= \rho \nabla_x \varphi \\ \partial_t W + \nabla_x \cdot ((W + p)U) &= \rho U \cdot \nabla_x \varphi \\ \nabla_x \varphi &= \rho - 1 \end{aligned}$$

where

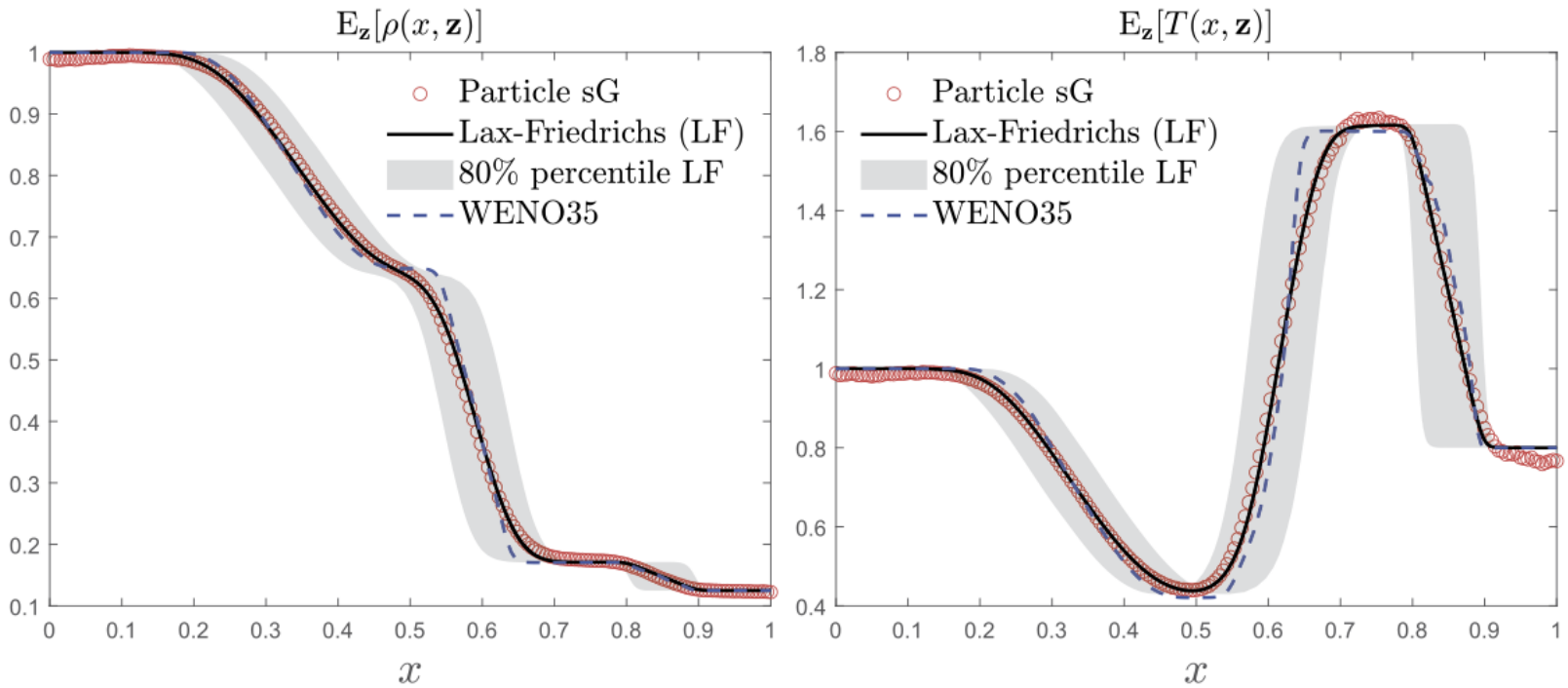
$$\rho = \rho(\mathbf{z}, x, t) = \int_{\mathbb{R}^{d_v}} f(\mathbf{z}, x, v, t) dv, \qquad \rho U = \rho U(\mathbf{z}, x, t) = \int_{\mathbb{R}^{d_v}} v f(\mathbf{z}, x, v, t) dv$$

and $T(\mathbf{z}, x, t) = \frac{1}{3\rho} \int_{\mathbb{R}^{d_v}} |v - U(\mathbf{z}, x, t)|^2 f(\mathbf{z}, x, v, t) dv$ defining

$$W(\mathbf{z}, x) = \rho(\mathbf{z}, x, t) \left(\frac{|U(\mathbf{z}, x, t)|^2}{2} + \frac{3T(\mathbf{z}, x, t)}{2} \right), \qquad p(\mathbf{z}, x, t) = \rho T.$$

Euler-Poisson equation with uncertainties

A direct application of sG methods to the Euler-Poisson system would lead to the loss of hyperbolicity of the problem. [14] On the other hand, thanks to the introduced particle Galerkin method we guarantee the conservation of hyperbolicity (due to reconstruction of the density in the phase space) together with relaxation towards local Maxwellian. [15].



[14] B.Despres, G. Poëtte, D. Lucor

[15] A. Medaglia, L.Pareschi, M.Z. '23

Conclusion

- To mimic the effects of missing information on the model parameters or initial conditions we need to include uncertainties on the parameters characterizing the system of interest.
- UQ imposes development of new schemes. We may considered Stochastic Galerkin methods, that are spectrally accurate in the random field but may lead to the loss of important structural properties of the numerical solution of kinetic equations.
- We have developed a robust and accurate approach that can effectively capture the behaviour of charged particles in collisional plasmas under uncertain data. The development of stochastic Galerkin particle methods allows to guarantee physical properties of the solution together with accuracy in terms of random quantities.
- The propagation of regularity should be investigated carefully.
- **Future research directions**
  - sG for the non-homogeneous Boltzmann and Landau
  - regularity for the Landau equation and its particle approximation
  - ...

Some references

- L. Pareschi, M. Zanella. Monte Carlo stochastic Galerkin methods for the Boltzmann equation with uncertainties: Space-homogeneous case. *J. Comput. Phys.*, 423:109822, 2020.
- A. Medaglia, L. Pareschi, M. Zanella. Stochastic Galerkin particle methods for kinetic equations of plasmas with uncertainties. *J. Comput. Phys.*, 479:112011, 2023.
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- R. Bailo, J.A. Carrillo, A. Medaglia, M. Zanella. Particle Galerkin methods for the homogeneous Landau equation as a gradient flow. In preparation.