PRIN 2017 Workshop on
Innovative Numerical Methods for Evolutionary Partial Differential Equations and Applications
(In memory of Maurizio)

Stochastic Galerkin particle methods
for kinetic equations with uncertainties

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Research group

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Main research topics

- AP methods for kinetic equations (plasma, rarefied gases) [WP1, WP3]
- Semi-lagrangian IMEX schemes, all Mach flows [WP2, WP4]
- PDEs on networks (epidemiology, blood flows) [WP5]
- Mean-field optimization and optimal control [WP7]
- Uncertainty quantification [WP9]
Uncertainty quantification

Physical, biological, social, economic etc. systems often involve uncertainties which should be accounted for in the mathematical models describing these systems.
Uncertainty quantification in PDEs

- Examples include uncertainty in the initial data, the boundary conditions, or in the modeling parameters like microscopic interactions, external forces, viscosity coefficient, ...  

- Need of constructing effective numerical methods for uncertain kinetic models and to analyze the new algorithms (Curse of dimensionality).

- Quantify uncertainties on some quantity of interest, like expected values and variance of moments.
## Uncertainty quantification approaches

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\(^1\) B.Peherstorfer, K.Willcox, M.Gunzburger, ’18; G.Dimarco, L.P. ’19-’20; L.Liu, L.P., X.Zhu ’20-’22;

\(^2\) S.Jin, J.Hu, L.Liu, R.Shu, Y.Zhu, ...., ’16-’20; T.Xiao, M.Frank ’21

\(^3\) S.Mishra, C.Schwab ’12; B.Despres, B.Perthame ’16; J.Hu, L.P., Y.Wang ’21; J.Hu, S.Jin, J.Li, L.Zhang ’22
Stochastic Galerkin particle methods

**Main idea:** combine accuracy of stochastic Galerkin methods in random space with efficiency of particle methods in phase space\(^4\).

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Classical sG approach (left branch) based on finite differences/volumes versus sG particle approach (right branch).

We consider the evolution of the plasma electrons at the kinetic level

\[
\frac{\partial f(x, v, t, z)}{\partial t} + v \cdot \nabla_x f(x, v, t, z) + E(x, t, z) \cdot \nabla_v f(x, v, t, z) = \frac{1}{\varepsilon} Q(f, f)(x, v, t, z).
\]

\(\varepsilon\) Knudsen number, \(z \in \Omega\) random vector \(\sim p(z)\), \(E(x, t, z)\) self-consistent electric field

\[
E(x, t, z) = -\nabla_x \phi(x, t, z),
\]

where \(\phi(x, t, z)\) is the potential, solution to the Poisson equation

\[
\Delta_x \phi(x, t, z) = 1 - \int_{\mathbb{R}^3} f(x, v, t, z) dv.
\]

\(Q(f, f)\) describes interactions between charged particles and is given by the Landau operator

\[
Q(f, f)(x, v, t, z) = \nabla_v \cdot \int_{\mathbb{R}^{d_v}} A(v - v_*, z) [\nabla_v f(v, z)f(v_*, z) - \nabla_{v_*} f(v_*, z)f(v, z)] dv_*,
\]

with \(A(v - v_*, z)\) a \(d_v \times d_v\) symmetric matrix characterizing the Coulombian interactions.
Asymptotic behaviors

In the collisionless case $\varepsilon \to +\infty$ we recover the Vlasov-Poisson system.

In the fluid-limit $\varepsilon \to 0$ from $Q(f, f) = 0$ we obtain $f = M_{\rho, U, T}$ with

$$M_{\rho, U, T}(x, v, t, z) = \rho(x, t, z) \left( \frac{1}{2\pi T(x, t, z)} \right)^{d_v/2} \exp \left( -\frac{(v - U(x, t, z))^2}{2T(x, t, z)} \right),$$

$$\rho(x, t, z) = \int_{\mathbb{R}^d} f \, dv, \quad U(x, t, z) = \frac{1}{\rho} \int_{\mathbb{R}^d} f v \, dv, \quad T(x, t, z) = \frac{1}{d_v \rho} \int_{\mathbb{R}^d} f (v - U)^2 \, dv,$$

the uncertain mass, momentum and temperature. Thus, defining

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

we recover the uncertain Euler-Poisson system

$$\partial_t \rho + \nabla_x \cdot (\rho U) = 0$$
$$\partial_t (\rho U) + \nabla_x \cdot (\rho U \otimes U) + \nabla_x p = \rho \nabla_x \phi$$
$$\partial_t W + \nabla_x \cdot ((W + p) U) = \rho U \cdot \nabla_x \phi$$
$$\Delta_x \phi = \rho - 1.$$
Operator splitting approach

Denoting by \( f^n(x, v, z) \) an approximation of \( f(x, v, t^n, z) \), with \( t^n = n\Delta t \), we solve separately

\[
(C_{\Delta t}) \begin{cases}
\frac{\partial f^*}{\partial t} = \frac{1}{\varepsilon} Q(f^*, f^*), \\
f^*(x, v, 0, z) = f^n(x, v, z),
\end{cases}
\]

an homogeneous collision process, and the Vlasov-Poisson system

\[
(T_{\Delta t}) \begin{cases}
\frac{\partial f^{**}}{\partial t} + v \cdot \nabla_x f^{**} + E(x, t, z) \cdot \nabla_v f^{**} = 0, \\
f^{**}(x, v, 0, z) = f^*(x, v, \Delta t, z).
\end{cases}
\]

The solution at the time \( t^{n+1} \) is therefore given by \( f^{n+1}(x, v, z) = f^{**}(x, v, \Delta t, z) \).

Higher order splitting techniques can be adopted, like the second order Strang splitting 5.

In the sequel we consider the simplified case of a BGK collision term

\[
Q(f, f)(x, v, t, z) = \nu(M_{\rho, U, T}(x, v, t, z) - f(x, v, t, z)),
\]

where \( \nu > 0 \) is the collision frequency.

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5G. Strang '68
The particle method in absence of uncertainties

Monte Carlo method for the collision step

We rewrite the collision step as the explicit solution

\[
    f^*(x, v) = \exp\left(-\nu \frac{\Delta t}{\varepsilon}\right) f^n(x, v) + \left(1 - \exp\left(-\nu \frac{\Delta t}{\varepsilon}\right)\right) M_{\rho, U, T}(x, v).
\]

**no collision** \quad **Maxwellian sampling**

Probabilistic interpretation: with probability \(1 - e^{-\nu \Delta t/\varepsilon}\) a particle’s velocity is replaced with a Maxwellian \(M_{\rho, U, T}\) sample. The sampling is made conservative by the shift and scale technique\(^6\).

The macroscopic quantities \(\rho^n_{\ell}, u^n_{\ell}\) and \(T^n_{\ell}\) are reconstructed in the cell \(I_{\ell}\), \(\ell = 1, \ldots, L\).

\(^6\)L. Pareschi, S. Trazzi ’05; D. Pullin ’80
The particle method in absence of uncertainties

**Particle in Cell method for the Vlasov-Poisson step**

The equations of motion of the particles are the following coupled set of ODEs

\[
\frac{dx_i(t)}{dt} = v_i(t), \quad \frac{dv_i(t)}{dt} = E(x_i, t).
\]

Let \( E_{n+1/2}^n \) be the electric field in the cell \( I_\ell \) at time \( t^{n+1/2} \). The particle dynamic is solved on the computational domain through the following Verlet type scheme

\[
x_i^{n+1/2} = x_i^n + v_i^n \frac{\Delta t}{2},
\]

\[
v_i^{n+1} = v_i^n + \Delta t \sum_{\ell=1}^{N_\ell} E_{n+1/2}^n \chi(x_i^{n+1/2} \in I_\ell),
\]

\[
x_i^{n+1} = x_i^{n+1/2} + v_i^{n+1} \frac{\Delta t}{2}.
\]

The electric field is computed by solving the Poisson equation for the potential with a mesh based method on a uniform staggered grid with respect to the cells \( I_\ell, \ell = 1, \ldots, L \).

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7E. Sonnendrücker ’13; P. Degond, F. Deluzet, L. Navoret, A. Sun, M. Vignal ’10; F. Filbet, L. Rodrigues ’16
Stochastic Galerkin (sG) particle methods

We consider the uncertain particles dynamic \((x_i(t, z), v_i(t, z)), i = 1, \ldots, N\) at time \(t\) with \(z \sim p(z)\), one-dimensional random variable.

Approximate uncertain position and velocities by generalized polynomial chaos (gPC) expansions\(^8\)

\[
x_i(t, z) \approx x_i^M(t, z) = \sum_{h=0}^{M} \hat{x}_{i,h}(t) \Psi_h(z), \quad v_i(t, z) \approx v_i^M(t, z) = \sum_{h=0}^{M} \hat{v}_{i,h}(t) \Psi_h(z),
\]

\(\{\Psi_h(z)\}_{h=0}^M\) set of polynomials of degree \(\leq M\), orthonormal with respect to \(p(z)\).

\(^8\)N. Wiener '38; D. Xiu, G. Karniadakis '02; J. Carrillo, L. Pareschi, M. Zanella '18, A. Medaglia, L. Pareschi, M. Zanella '22
The sG particle projection

By orthogonality

$$\int_{\Omega} \Psi_h(z) \Psi_k(z) p(z) dz = E_z [\Psi_h(\cdot) \Psi_k(\cdot)] = \delta_{hk},$$

$$\Omega \subseteq \mathbb{R}^d$$ and $$\delta_{hk}$$ is the Kronecker delta.

The coefficients $$\hat{x}_{i,h}(t)$$ and $$\hat{v}_{i,h}(t)$$ are projections in the space of polynomials of degree $$h \geq 0$$

$$\hat{x}_{i,h} = \int_{\Omega} x_i(z) \Psi_h(z) p(z) dz = E_z [x_i^n(\cdot) \Psi_h(\cdot)], \quad \hat{v}_{i,h} = \int_{\Omega} v_i(z) \Psi_h(z) p(z) dz = E_z [v_i^n(\cdot) \Psi_h(\cdot)].$$

Let $$H^r(\Omega)$$ be a weighted Sobolev space

$$H^r(\Omega) = \left\{ u : \Omega \rightarrow \mathbb{R} : \frac{\partial^k u}{\partial z^k} \in L^2(\Omega), 0 \leq k \leq r \right\}.$$

Lemma (Spectral accuracy)

For any $$u(z) \in H^r(\Omega), r \geq 0$$, there exists a constant $$C$$ independent of $$M > 0$$ such that

$$\|u - u^M\|_{L^2(\Omega)} \leq \frac{C}{M^r} \|u\|_{H^r(\Omega)},$$
sG particle method for plasmas

sG collision step

Rewrite the Monte Carlo method in compact form to insert the gPC expansions $x_{i}^{M,n}(z), v_{i}^{M,n}(z)$

$$v_{i}^{M,n+1}(z) = \chi \left( \xi < e^{-\nu \Delta t} \right) v_{i}^{M,n}(z) + \left( 1 - \chi \left( \xi < e^{-\nu \Delta t} \right) \right) \sum_{\ell=1}^{L} \chi \left( x_{i}^{M,n}(z) \in I_{\ell} \right) \tilde{v}_{\ell}^{M}(z)$$

$\chi(\cdot)$ is the indicator function, $\xi \sim \mathcal{U}([0,1])$ and $\tilde{v}_{\ell}^{M}(z)$ a sample from $\mathcal{M}_{\rho_{\ell}^{M,n}(z), U_{\ell}^{M,n}(z), T_{\ell}^{M,n}(z)}$.

Projecting the above equation for each $h = 0, \ldots, M$ we get

$$\hat{v}_{i,h}^{n+1} = \chi \left( \xi < e^{-\nu \Delta t} \right) \hat{v}_{i,h}^{n} + \left( 1 - \chi \left( \xi < e^{-\nu \Delta t} \right) \right) \sum_{\ell=1}^{L} \hat{W}(t_{i,h}^{n})_{\ell}$$

$$\hat{W}(t_{i,h}^{n})_{\ell} = \int_{\Omega} \chi \left( x_{i}^{M,n}(z) \in I_{\ell} \right) \tilde{v}_{\ell}^{M}(z) \Psi_h(z)p(z)dz,$$

and the above integral is computed through Gaussian quadrature with $M$ nodes.
sG particle method for plasmas

sG Vlasov-Poisson step

The gPC expansion of the particles’ systems \( x_i^M(t, z), v_i^M(t, z) \) is solution to

\[
\frac{dx_i^M(t, z)}{dt} = v_i^M(t, z), \quad \frac{dv_i^M(t, z)}{dt} = E^M(x_i^M, t, z).
\]

Hence, we project the latter set of ODEs in the linear space \( \{ \Psi_h(z) \}_{h=0}^M \) to obtain

\[
\frac{d\hat{x}_{i,h}(t)}{dt} = \hat{v}_{i,h}(t), \quad \frac{d\hat{v}_{i,h}(t)}{dt} = \int_\Omega E^M(x_i^M, t, z) \Psi_h(z)p(z)dz.
\]

The projected time discretized scheme then reads

\[
\hat{x}_{i,h}^{n+1/2} = \hat{x}_{i,h}^n + \hat{v}_{i,h}^n \Delta t/2,
\]

\[
\hat{v}_{i,h}^{n+1} = \hat{v}_{i,h}^n + \Delta t \sum_{\ell=1}^{N_\ell} \int_\Omega E_{\ell}^{n+1/2,M}(z) \chi(x_{i,h}^{n+1/2,M}(z) \in I_\ell) \Psi_h(z)p(z)dz,
\]

\[
\hat{x}_{i,h}^{n+1} = \hat{x}_{i,h}^{n+1/2} + \hat{v}_{i,h}^{n+1} \Delta t/2.
\]

The electric field needs to be calculated for every Gaussian node used in the quadrature.
Neglecting for simplicity space dependence, given a function \( f(z,v,t) \) approximated by samples, its empirical measure and the sG empirical measure are

\[
f^N(z,v,t) = \frac{1}{N} \sum_{i=1}^{N} \delta(v - v_i(z,t)), \quad f^N_M(z,v,t) = \frac{1}{N} \sum_{i=1}^{N} \delta(v - v_i^M(z,t)).
\]

For any a test function \( \varphi \), if we denote by

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

we have

\[
\langle \varphi, f^N \rangle(z,t) = \frac{1}{N} \sum_{i=1}^{N} \varphi(v_i(z,t)), \quad \langle \varphi, f^N_M \rangle(z,t) = \frac{1}{N} \sum_{i=1}^{N} \varphi(v_i^M(z,t)).
\]

Assuming \( \int_{\mathbb{R}^d} f(z,v,t) \, dv = 1 \), then \( \langle \varphi, f \rangle(z,t) \) is the expectation of \( \varphi \) with respect to \( f \), that we denote as \( \mathbb{E}_V[\varphi](z) \). Similarly, we denote by \( \sigma^2_{\varphi}(z) = \text{Var}_V(\varphi)(z) \) its variance with respect to \( f \).
For a random variable $V(z,t)$ taking values in $L^2(\Omega)$ we define

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

For each $z \in \Omega$, $\langle \varphi, f^N \rangle(z,t)$ is the sum of $N$ random variables $\varphi(v_1(z,t)), \ldots, \varphi(v_N(z,t))$ with $v_1(z,t), \ldots, v_N(z,t)$ i.i.d. as $f(z,v,t)$.

We have the following consistency estimate \(^9\)

**Theorem**

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

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

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

\(^9\)L.P., M. Zanella ’19
Test 1: spectral convergence

$L^2$ error of the sG particle scheme in the collisionless case $N = 10^6$, $\Delta t = 0.1$ and a reference solution with $M = 30$. We choose a random initial temperature $T(z) = \frac{4}{5} + \frac{2}{5}z$, $z \sim U([0, 1])$ and initial data

$$f_0(x, v, z) = \rho(x) \frac{1}{\sqrt{2\pi T(z)}} e^{-\frac{v^2}{2T(z)}}, \quad \rho(x) = \frac{1}{\sqrt{\pi}} e^{-(x-6)^2}, \quad x \in [0, 4\pi]$$
Test 2: Landau damping

We consider a wave perturbation of the local Maxwellian distribution. If the perturbation is small, we are in the so-called linear Landau damping regime, if the wave amplitude increases, we get the nonlinear Landau damping regime.

Initial data is an uncertain perturbation of the local equilibrium

\[ f_0(x, v, z) = (1 + \alpha(z) \cos(\kappa x)) \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}, \]

with \( x \in [0, 2\pi/k], \ v \in [-6, 6], \ \kappa \) the wave number and \( \alpha(z) \) small random perturbation.

The \( L^2 \)-norm of the electric field

\[ \mathcal{E}(t, z) = \left( \int_{\mathbb{R}^3} \left| E(x, t, z) \right|^2 dx \right)^{\frac{1}{2}} \]

decays at a specific damping rate \( \gamma \). In the collisionless case we have explicit expressions for \( \gamma \) in the linear case, and of the damping and growth rates \( \gamma_d \) and \( \gamma_g \) in the nonlinear case\(^{10}\).

\(^{10}\)F.F.Chen, ’74, F.Filbet, T.Xiong ’22
Linear Landau damping \((\alpha(z) \sim \mathcal{U}([0.05, 0.15]))\)
Nonlinear Landau damping \( (\alpha(z) \sim U([0.4, 0.6])) \)
Logarithm of $\log (E_{z}[\mathcal{E}(t, z)])$. Linear (top) and nonlinear (bottom) Landau damping. From left to right: $\varepsilon = +\infty$, $\varepsilon = 1$, $\varepsilon = 10^{-3}$. The wave number is $\kappa = 0.5$. For $\varepsilon = +\infty$ we have $\gamma = -0.1533$ (linear) and $\gamma_d = -0.2920$, $\gamma_g = 0.0815$ (nonlinear). Here $N = 10^7$, $M = 5$, $\Delta t = 0.1$. 

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Lorenzo Pareschi

Stochastic Galerkin particle methods for multiscale collisional plasmas with uncertainties
Test 3: Two stream instability

For the two stream instability we consider the initial distribution\textsuperscript{11}

\[ f_0(x, v, z) = (1 + \alpha(z) \cos(\kappa x)) \frac{1}{2\sqrt{2\pi T}} \left( e^{-\frac{(v-\bar{v})^2}{2T}} + e^{-\frac{(v+\bar{v})^2}{2T}} \right). \]

We take \( x \in [0, 2\pi/k] \) and \( v \in [-L_v, L_v] \), with \( L_v = 6 \).

- To observe the linear two stream instability we take \( \bar{v} = 2.4, T = 1 \), a wave number \( \kappa = 0.2 \).
  In the collisionless scenario, if the random perturbation is small, after a certain amount of time the logarithm of the \( L^2 \)-norm of the electric energy grows linearly with a specific rate \( \gamma \).

- In the nonlinear two stream instability we choose \( \bar{v} = 0.99, T = 0.3 \), a wave number \( \kappa = 2/13 \). In this case due to the effect of collisions the instabilities disappear.

\textsuperscript{11}F. Filbet, E. Sonnendr{"u}cker '01
Linear two stream instability \( \alpha(z) \sim U([0.003, 0.007]) \)
Nonlinear two stream instability \( \alpha(z) \sim \mathcal{U}([0.04, 0.06]) \)
Nonlinear two stream instability ($\varepsilon = 1$)
Test 4: Sod shock tube (uncertain temperature, $\varepsilon = 10^{-3}$)

Sod shock tube with uncertain initial temperature $T_0(x,z) = 1 + z/4$, $z \sim U([0,1])$. The particle sG solution is computed with $N = 10^7$, $M = 5$ and $\Delta t = 0.01$. Euler-Poisson: Lax-Friedrichs is solved with 1500 cells, WENO with 200 cells and stochastic collocation with 11 nodes.
Sod shock tube with uncertain initial shock position \( x^* = 0.5 + \alpha(z), \; \alpha(z) = -0.05 + 0.1z, \; z \sim U([0, 1]). \) The particle sG solution is computed with \( N = 10^7, \; M = 5 \) and \( \Delta t = 0.01. \) Euler-Poisson: Lax-Friedrichs is solved with 1500 cells, WENO with 200 cells and stochastic collocation with 11 nodes.
Concluding remarks

• **Stochastic Galerkin (sG) particle methods** combine an efficient particle solver in the physical space with an accurate sG method in the random space.

• For **smooth solutions** in the random space, very few modes are sufficient to match the particle accuracy in the physical space ($M \ll N$).

• They preserve the main properties of the solution such as physical conservations and non negativity and avoid loss of hyperbolicity of sG methods for systems of conservation laws.

• Some research directions involve
  
  • inclusion of Landau collision effects\(^\text{12}\)
  • study of the convergence properties
  • inclusion of the magnetic field
  • analysis of the boundary conditions
  • ...

\(^{12}\)A. Medaglia, L.P., M. Zanella '23