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

Lorenzo Pareschi

Department of Mathematics and Computer Science, University of Ferrara, Italy

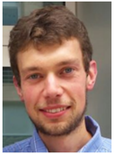
February 20-22, 2023 — University of Catania

PRIN 2017: The research unit of Ferrara

Research group


L. Pareschi


G. Dimarco


W. Boscheri


V. Caleffi


A. Valiani

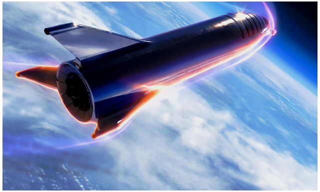

G. Bertaglia

Main research topics

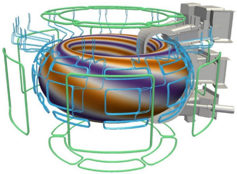
- AP methods for kinetic equations (plasma, rarefied gases) [WP1, WP3]
- Semi-lagrangian IMEX schemes, all Mach flows [WP2, WP4]
- PDEs on networks (epidemiology, blood flows) [WP5]
- Mean-field optimization and optimal control [WP7]
- Uncertainty quantification [WP9]

Uncertainty quantification

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

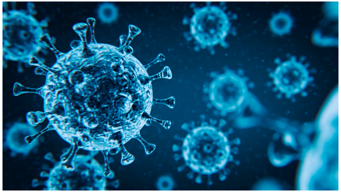


Reentry problem

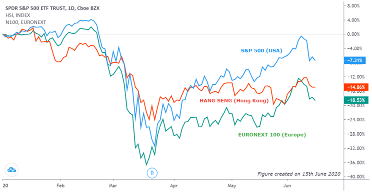


Plasma fusion

Traffic flow



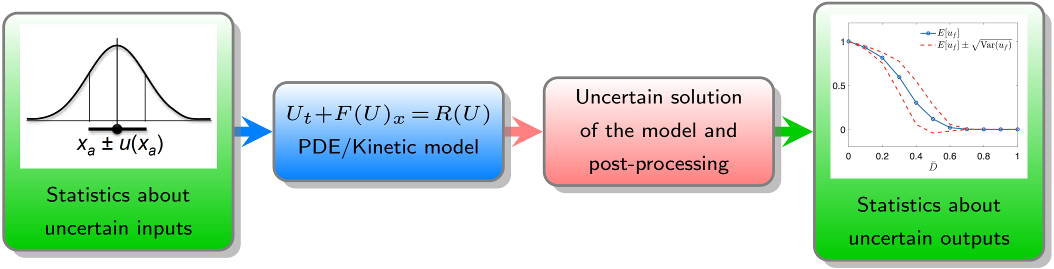
Covid-19



Finance

Collective behavior

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

Multifidelity	accelerate Monte Carlo sampling using different fidelity models[1]. Model dependent but very efficient (non-intrusive) for high dimensional random spaces. Properties of the underlying solver.
Stochastic Galerkin (sG)	generalized polynomial chaos (gPC) expansions in the random space and deterministic methods in physical space[2]. Spectral accuracy, high cost (intrusive), loss of physics, hyperbolicity.
Other methods	designed for uncertainty quantification, like Moment methods, Kinetic polynomials, Multilevel Monte Carlo methods, ...[3]

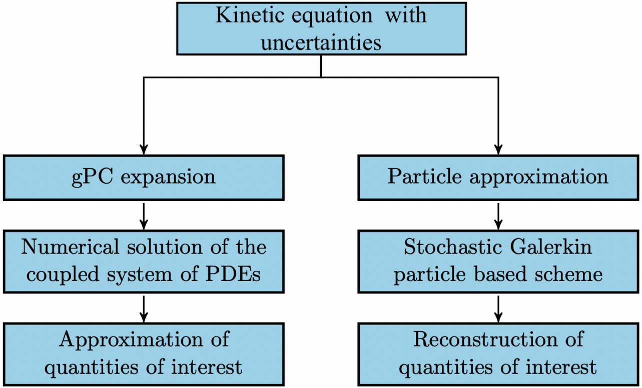
[1] B.Peherstorfer, K.Willcox, M.Gunzburger, '18; G.Dimarco, L.P. '19-'20; L.Liu, L.P., X.Zhu '20-'22;

[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].



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

[4] J.Carrillo, L.P., M.Zanella '18; G. Poëtte '19; L.P., M.Zanella '21; A.Medaglia, L.P., M.Zanella '22

Kinetic models of plasmas with uncertainties

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

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

ε 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

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

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 $f = \mathcal{M}_{\rho,U,T}$ with

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

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

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

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

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

$$(\mathcal{C}_{\Delta t}) \begin{cases} \dfrac{\partial f^*}{\partial t} = \dfrac{1}{\varepsilon} Q(f^*, f^*), \\ f^*(x,v,0,z) = f^n(x,v,z), \end{cases}$$

an homogeneous collision process, and the Vlasov-Poisson system

$$(\mathcal{T}_{\Delta t}) \begin{cases} \dfrac{\partial f^{**}}{\partial t} + v \cdot \nabla_x f^{**} + E(x,t,z) \cdot \nabla_v f^{**} = 0, \\ f^{**}(x,v,0,z) = f^*(x,v,\Delta t,z). \end{cases}$$

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

$$Q(f,f)(x,v,t,z) = \nu(\mathcal{M}_{\rho,U,T}(x,v,t,z) - f(x,v,t,z)),$$

where $\nu > 0$ is the collision frequency.

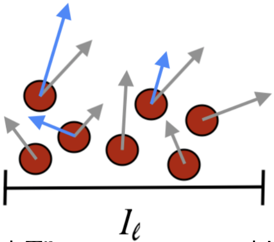
[5] G. Strang '68

Monte Carlo method for the collision step

We rewrite the collision step as the explicit solution

$$f^*(x,v) = \underbrace{\exp\left(-\nu\frac{\Delta t}{\varepsilon}\right) f^n(x,v)}_{\text{no collision}} + \underbrace{\left(1-\exp\left(-\nu\frac{\Delta t}{\varepsilon}\right)\right) \mathcal{M}_{\rho,U,T}(x,v)}_{\text{Maxwellian sampling}}.$$

Probabilistic interpretation: with probability $1-e^{-\nu\Delta t/\varepsilon}$ a particle's velocity is replaced with a Maxwellian $\mathcal{M}_{\rho,U,T}$ sample. The sampling is made conservative by the shift and scale technique[6].



The macroscopic quantities ρ_ℓ^n, u_ℓ^n and T_ℓ^n are reconstructed in the cell I_ℓ, $\ell = 1,\ldots,L$.

[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[7]

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

$$\frac{dx_i(t)}{dt} = v_i(t), \qquad \frac{dv_i(t)}{dt} = E(x_i, t).$$

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

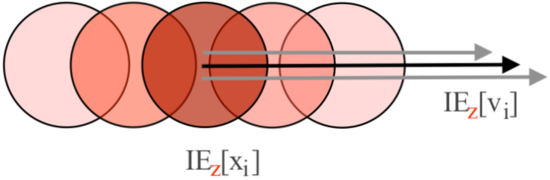
$$\begin{aligned} x_i^{n+1/2} &= x_i^n + v_i^n \frac{\Delta t}{2}, \\ v_i^{n+1} &= v_i^n + \Delta t \sum_{\ell=1}^{N_\ell} E_\ell^{n+1/2} \chi(x_i^{n+1/2} \in I_\ell), \\ x_i^{n+1} &= x_i^{n+1/2} + v_i^{n+1} \frac{\Delta t}{2}. \end{aligned}$$

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_ℓ, $\ell = 1, \ldots, L$.

[7] E. 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 $(x_i(t,z), v_i(t,z))$, $i = 1,\dots,N$ at time t with $z \sim p(z)$, one-dimensional random variable.



Approximate uncertain position and velocities by generalized polynomial chaos (gPC) expansions[8]

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

$\{\Psi_h(z)\}_{h=0}^M$ 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

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

$\Omega \subseteq \mathbb{R}^d$ and δ_{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 $h \geq 0$

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

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

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

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 $x_i^{M,n}(z)$, $v_i^{M,n}(z)$

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

$\chi(\cdot)$ 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

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

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

and the above integral is computed through Gaussian quadrature with M nodes.

sG Vlasov-Poisson step

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

$$\frac{dx_i^M(t, z)}{dt} = v_i^M(t, z), \qquad \frac{dv_i^M(t, z)}{dt} = E^M(x_i^M, t, z).$$

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

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

The projected time discretized scheme then reads

$$\begin{aligned} \hat{x}_{i,h}^{n+1/2} &= \hat{x}_{i,h}^{n} + \hat{v}_{i,h}^{n}\Delta t/2, \\ \hat{v}_{i,h}^{n+1} &= \hat{v}_{i,h}^{n} + \Delta t \sum_{\ell=1}^{N_\ell} \int_\Omega E_\ell^{n+1/2,M}(z)\chi(x_i^{n+1/2,M}(z) \in I_\ell)\Psi_h(z)p(z)dz, \\ \hat{x}_{i,h}^{n+1} &= \hat{x}_{i,h}^{n+1/2} + \hat{v}_{i,h}^{n+1}\Delta t/2. \end{aligned}$$

The electric field needs to be calculated for every Gaussian node used in the quadrature.

Error estimate on moments

Neglecting for simplicity space dependence, given a function $f(z,v,t)$ approximated by samples, its empirical measure and the sG empirical measure are

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

For any a test function φ, if we denote by

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

we have

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

Assuming $\int_{\mathbb{R}^d} f(z,v,t)\,dv = 1$, then $\langle \varphi, f\rangle(z,t)$ is the expectation of φ with respect to f, that we denote as $\mathbb{E}_V[\varphi](z)$. Similarly, we denote by $\sigma^2_\varphi(z) = \mathrm{Var}_V(\varphi)(z)$ 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 $\varphi(v_1(z,t)),\dots,\varphi(v_N(z,t))$ with $v_1(z,t),\dots,v_N(z,t)$ i.i.d. as $f(z,v,t)$.

We have the following consistency estimate [9]

Theorem

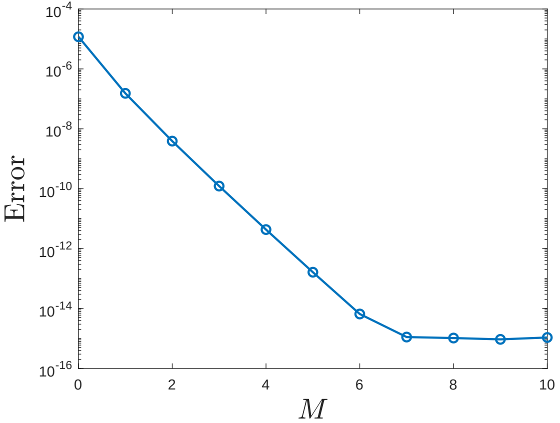
Let $f(z,v,t)$ a probability density function in v at time $t \geq 0$ and $f_M^N(z,v,t)$ the empirical measure of the N-particles sG approximation with M projections associated to the samples $\{v_1(z,t),\dots,v_N(z,t)\}$. Provided that $v_i(z,t) \in H^r(\Omega)$ for all $i = 1,\dots,N$, we have

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

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

[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 $T(z) = \frac{4}{5} + \frac{2}{5}z$, $z \sim \mathcal{U}([0,1])$ and initial data

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

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

The L^2-norm of the electric field

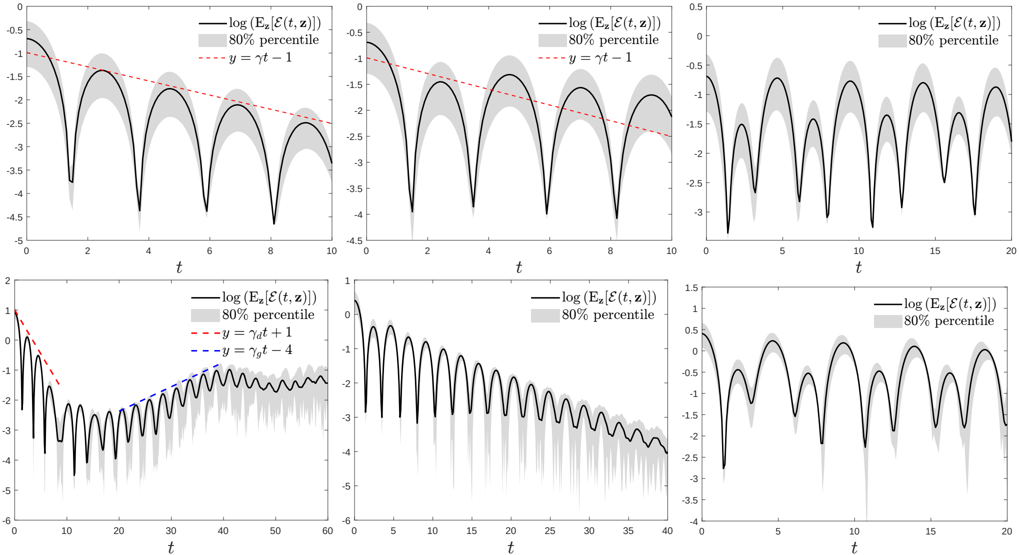
$$\mathcal{E}(t, z) = \left(\int_{\mathbb{R}^3} |E(x, t, z)|^2 dx\right)^{\frac{1}{2}}$$

decays at a specific damping rate γ. In the collisionless case we have explicit expressions for γ in the linear case, and of the damping and growth rates γ_d and γ_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 ($\alpha(z) \sim \mathcal{U}([0.4, 0.6])$)



Logarithm of $\mathbb{E}_z[\mathcal{E}(t,z)]$. 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 $N=10^7$, $M=5$, $\Delta t=0.1$.

Test 3: Two stream instability

For the two stream instability we consider the initial distribution[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 γ.

- 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.

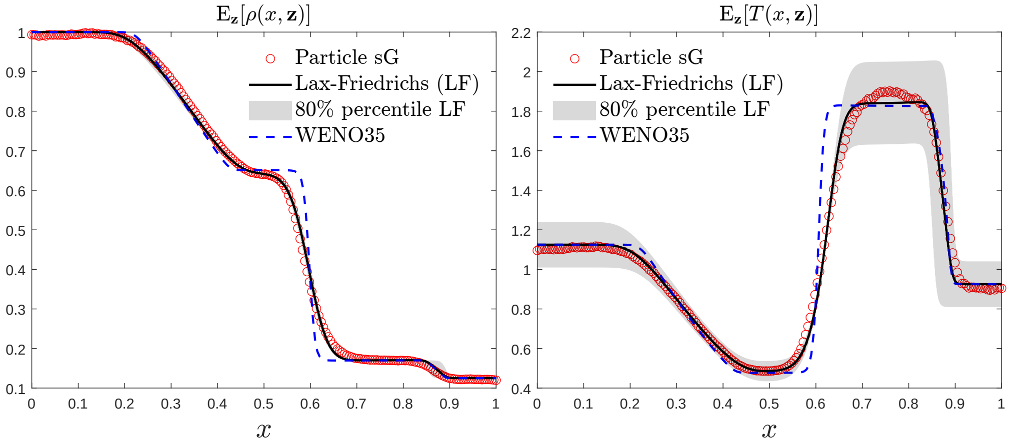
[11] F.Filbet, E.Sonnendrücker '01

Linear two stream instability ($\alpha(z) \sim \mathcal{U}([0.003, 0.007])$)

Nonlinear two stream instability ($\alpha(z) \sim \mathcal{U}([0.04, 0.06])$)

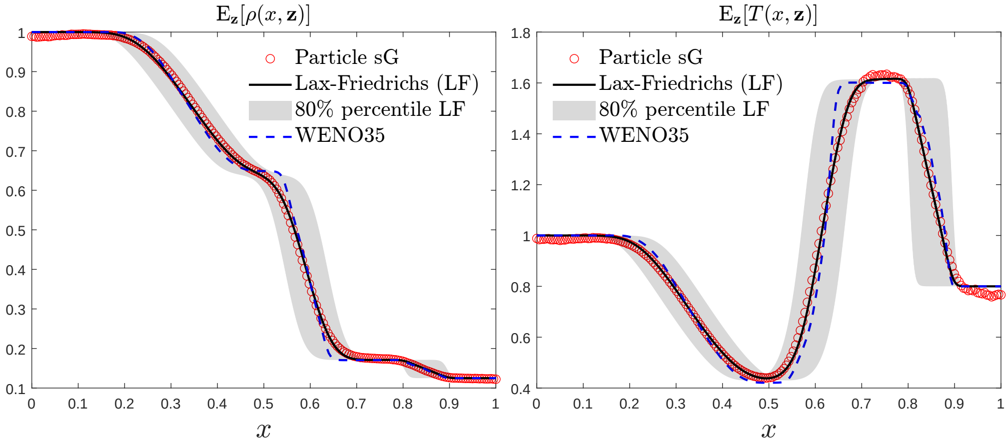
Nonlinear two stream instability ($\varepsilon = 1$)

Test 4: Sod shock tube (uncertain temperature, $\varepsilon = 10^{-3}$)



Sod shock tube with uncertain initial temperature $T_0(x, z) = 1 + z/4$, $z \sim \mathcal{U}([0, 1])$. 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.

Test 4: Sod shock tube (uncertain interface, $\varepsilon = 10^{-3}$)



Sod shock tube with uncertain initial shock position $x_* = 0.5 + \alpha(z)$, $\alpha(z) = -0.05 + 0.1z$, $z \sim \mathcal{U}([0,1])$. 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[12]
  - study of the convergence properties
  - inclusion of the magnetic field
  - analysis of the boundary conditions
  - ...

[12] A. Medaglia, L.P., M. Zanella '23