Uncertainty Quantification for multiscale kinetic equations with random inputs-II

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Uncertainty in kinetic equations

- Kinetic equations are usually derived from N-body Newton's second law, by mean-field limit, BBGKY hierachy, Grad-Boltzmann limit, etc.
- Collision kernels are often empirical
- Initial and boundary data contain uncertainties due to measurement errors or modelling errors; geometry, forcing
- While UQ has been popular in solid mechanics, CFD, elliptic equations, etc. there has been little effort for kinetic equation

UQ for kinetic models

For kinetic models, the only thing certain is their uncertainty

- Quantify the propagation of the uncertainty
- efficient numerical methods to study the uncertainty
- understand its statistical moments
- sensitivity analysis, long-time behavior of the uncertainty
- Control of the uncertainty
- dimensional reduction of high dimensional uncertainty
- …

Example: linear neutron transport with random cross-sections
(Jin-Xiu-Zhu JCP'14)

$$\epsilon\partial_t f(v) + v\partial_x f(v) = \frac{\sigma(x,z)}{\epsilon}\left[\frac{1}{2}\int_{-1}^{1} f(v')\,dv' - f(v)\right],$$

$\sigma(x,z)$ the scattering cross-section, is random

Diffusion limit: Larsen-Keller, Bardos-Santos-Sentis,
Bensoussan-Lions-Papanicolaou (for each z)

as $\epsilon \to 0^+$ f→ $\rho(t,x) = \frac{1}{2}\int_{-1}^{1} f(v')\,dv'$

$$\rho_t = \partial_x\left[\frac{1}{3\sigma(x,z)}\partial_x\rho\right]$$

Data for scattering cross-section

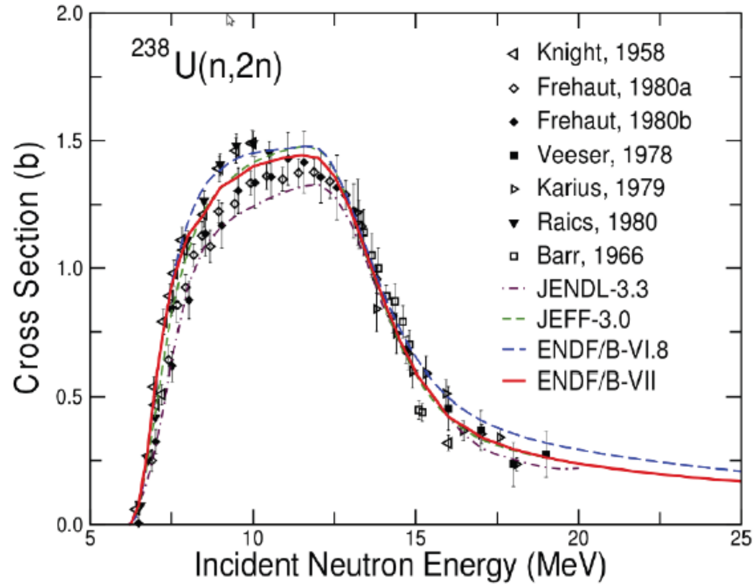


Figure 2: Example of uncertainty associated with a nuclear cross-section (from (Chadwick et al., 2006)). Figure contains values corresponding to several data libraries and measurements.

Some numerical methods for random PDEs

Sampling based methods (non-intrusive)

- The Monte-Carlo method (very efficient, no dimension curse, but only half-th order
- Stochastic collocation methods: using deterministic legacy code at well-chosen sample points, thus use interpolation or quadrature rules to get information at other random points or statistical moments

Stochastic Galerkin (Intrusive):

- Using polynomial chaos expansion plus Gelerkin projection: spectral method in the random space. Need to write a new code

Polynomial Chaos (PC) approximation

- The PC or generalized PC (gPC) approach first introduced by Wiener, followed by Cameron-Martin, and generalized by Ghanem and Spanos, Xiu and Karniadakis etc. has been shown to be very efficient in many UQ applications when the solution has enough regularity in the random variable
- Let z be a random variable with pdf $\rho(z) > 0$
- Let $\Phi_m(z)$ be the orthonormal polynomials of degree m corresponding to the weight $\rho(z) > 0$

$$\int \Phi_i(z)\Phi_j(z)\rho(z)\,dz = \delta_{ij}$$

The Wiener-Askey polynomial chaos for random variables (table from Xiu-Karniadakis SISC 2002)

	Random variables ζ	Wiener-Askey chaos $\{\Phi(\zeta)\}$	Support
Continuous	Gaussian	Hermite-Chaos	$(-\infty, \infty)$
	Gamma	Laguerre-Chaos	$[0, \infty)$
	Beta	Jacobi-Chaos	$[a, b]$
	Uniform	Legendre-Chaos	$[a, b]$
Discrete	Poisson	Charlier-Chaos	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk-Chaos	$\{0, 1, \dots, N\}$
	Negative Binomial	Meixner-Chaos	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn-Chaos	$\{0, 1, \dots, N\}$

TABLE 4.1

The correspondence of the type of Wiener-Askey polynomial chaos and their underlying random variables ($N \geq 0$ is a finite integer).

Generalized polynomial chaos stochastic Galerkin (gPC-sG) methods

- Take an orthonormal polynomial basis $\{\Phi_j(z)\}$ in the random space
- Expand functions into Fourier series and truncate:

$$f(z) = \sum_{j=0}^{\infty} f_j \phi_j(z) \approx \sum_{j=0}^{K} f_j \phi_j(z) := f^K(z).$$

- Substitute into system, Galerkin projection. Then one gets a deterministic system of the gPC coefficients $(f_0, \ldots, f_K)$

Accuracy and efficiency

- We will consider the gPC-stochastic Galerkin (gPC-SG) method
- Under suitable regularity assumptions this method has a spectral accuracy
- Much more efficient than Monte-Carlo samplings (halfth-order)
- Our regularity analysis is also important for stochastic collocation method

Stochastic AP schemes (s-AP)

2.1. Stochastic asymptotic preserving scheme. We now consider the same problem subject to random inputs.

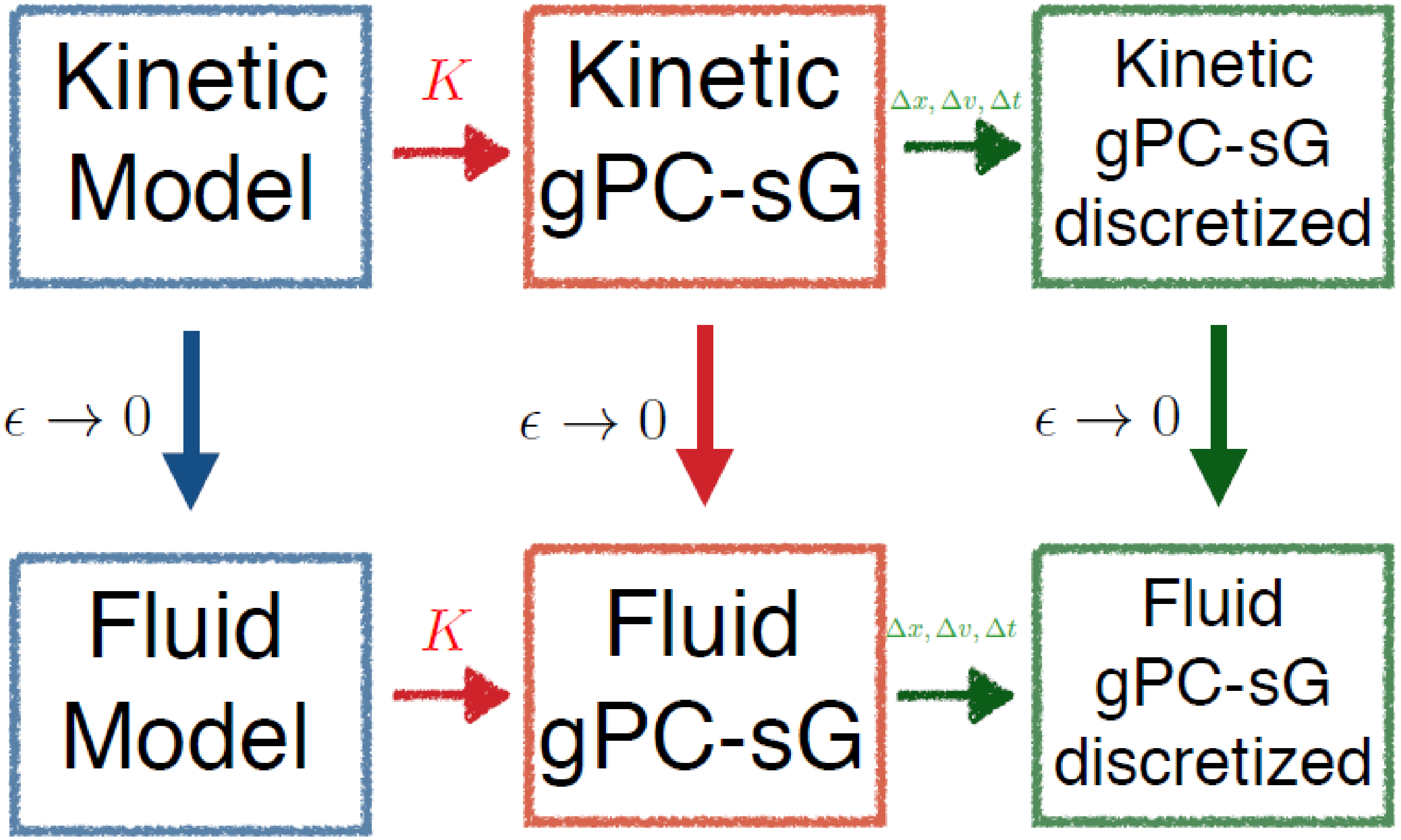
$$\partial_t u^\epsilon = \mathcal{L}^\epsilon(t, x, z, u^\epsilon; \epsilon), \tag{2.3}$$

where $z \in I_z \subseteq \mathbb{R}^d$, $d \geq 1$, are a set of random variables equipped with probability density function ρ. These random variables characterize the random inputs into the system. As $\epsilon \to 0$, the diffusive limit becomes

$$\partial_t u = \mathcal{L}(t, x, z, u). \tag{2.4}$$

We now extend the concept of deterministic AP to the stochastic case. To avoid the cluttering of notations, let us now focus on the discretization in the random space I_z.

DEFINITION 2.1 (Stochastic AP). *Let $\mathcal{S}$ be a numerical scheme for* (2.3), *which results in a solution $v^\epsilon(z) \in V_z$ in a finite dimensional linear function space V_z. Let $v(z) = \lim_{\epsilon \to 0} v^\epsilon(z)$ be its asymptotic limit. We say that the scheme $\mathcal{S}$ is* strongly asymptotic perserving *if the limiting solution $v(z)$ satisfies the limiting equation* (2.4) *for almost every $z \in I_z$; and it is* weakly asymptotic perserving *if the limiting solution $v(z)$ satisfies the limiting equation* (2.4) *in a weak form.*


Kinetic Model
K
Kinetic gPC-sG
Δx, Δv, Δt
Kinetic gPC-sG discretized
ε → 0
ε → 0
ε → 0
Fluid Model
K
Fluid gPC-sG
Δx, Δv, Δt
Fluid gPC-sG discretized

Linear transport equation with random coeffcients

$$\epsilon\partial_t f + v\partial_x f = \frac{\sigma(x,z)}{\epsilon}\left[\frac{1}{2}\int_{-1}^{1} f(v')\,dv' - f\right],$$

To understand its diffusion limit, we first split this equation into two equations for $v > 0$:

$$\begin{aligned}
\epsilon\partial_t f(v) + v\partial_x f(v) &= \frac{\sigma(x,z)}{\epsilon}\left[\frac{1}{2}\int_{-1}^{1} f(v')\,dv' - f(v)\right], \\
\epsilon\partial_t f(-v) - v\partial_x f(-v) &= \frac{\sigma(x,z)}{\epsilon}\left[\frac{1}{2}\int_{-1}^{1} f(v')\,dv - f(-v)\right],
\end{aligned} \tag{3.6}$$

and then consider its even and odd parities

$$\begin{aligned}
r(t,x,v) &= \frac{1}{2}[f(t,x,v) + f(t,x,-v)], \\
j(t,x,v) &= \frac{1}{2\epsilon}[f(t,x,v) - f(t,x,-v)].
\end{aligned} \tag{3.7}$$

Diffusion limit

The system (3.6) can then be rewritten as follows:

$$\begin{cases} \partial_t r + v\partial_x j = \dfrac{\sigma(x,z)}{\epsilon^2}(\overline{r} - r), \\ \partial_t j + \dfrac{v}{\epsilon^2}\partial_x r = -\dfrac{\sigma(x,z)}{\epsilon^2} j. \end{cases} \tag{3.8}$$

where

$$\overline{r}(t,x) = \int_0^1 r dv.$$

As $\epsilon \to 0^+$, (3.8) yields

$$r = \overline{r}, \qquad j = -\frac{v}{\sigma(x,z)}\partial_x \overline{r}.$$

Substituting this into system (3.8) and integrating over v, one gets the limiting diffusion equation ([23, 1]):

$$\partial_t \overline{r} = \partial_x \left[\frac{1}{3\sigma(x,z)} \partial_x \overline{r} \right]. \tag{3.9}$$

gPC approximations

$$r_N(x,z,t) = \sum_{m=1}^{M} \hat{r}_m(t,x)\Phi_m(z), \quad j_N(x,z,t) = \sum_{m=0}^{M} \hat{j}_m(t,x)\Phi_m(z) \tag{6.1}$$

be the Nth-order gPC expansion for the solutions and

$$\hat{\mathbf{r}} = (\hat{r}_1, \cdots, \hat{r}_M)^T, \quad \hat{\mathbf{j}} = (\hat{j}_1, \cdots, \hat{j}_M)^T,$$

$$\begin{cases} \partial_t \hat{\mathbf{r}} + v\partial_x \hat{\mathbf{j}} = \dfrac{1}{\epsilon^2}\mathbf{S}(x)(\overline{\mathbf{r}} - \hat{\mathbf{r}}), \\ \partial_t \hat{\mathbf{j}} + \dfrac{v}{\epsilon^2}\partial_x \hat{\mathbf{r}} = -\dfrac{1}{\epsilon^2}\mathbf{S}(x)\hat{\mathbf{j}}, \end{cases} \tag{6.2}$$

where

$$\overline{\mathbf{r}}(x,t) = \int_0^1 \hat{\mathbf{r}}\, dv,$$

and $\mathbf{S}(x) = (s_{ij}(x))_{1 \le i,j \le M}$ is a $M \times M$ matrix with entries

$$s_{ij}(x) = \int \sigma(x,z)\Phi_i(z)\Phi_j(z)\rho(z)\, dz. \tag{6.3}$$

Vectorized version of the deterministic problem (we can do APUQ!)

- One can now use deterministic AP schemes to solve this system

- Why s-AP?

- When $\epsilon \to 0$ the gPC-SG for transport equation becomes the gPC-SG for the limiting diffusion equation

gPC-SG for limiting diffusion equations

- For diffusion equation:

$$u_t = \partial_x[a(x,z)\partial_x u]$$

- Galerkin approximation:

$$u(x,z,t) = \sum_{m=0}^{M} \hat{u}_m(t,x)\Phi_m(z)$$

- moments: $\mathbb{E}[u] = \hat{u}_0\,,\qquad \mathrm{Var}[u] = \sum_{m=0}^{M} \hat{u}_m^2$
- Let $\hat{\mathbf{u}} = (\hat{u}_1, \cdots, \hat{u}_M)^T$ then

$$\partial_t \hat{\mathbf{u}} = \partial_x\left(\mathbf{A}\partial_x \hat{\mathbf{u}}\right) \qquad \mathbf{A} = (a_{ij})_{M\times M}$$ symm. pos. def

$$a_{ij}(x) = \int a(x,z)\Phi_i(z)\Phi_j(z)\rho(z)dz.$$

Uniform stability

- For a fully discrete scheme based on the deterministic micro-macro decomposition

  ($f=M + g$) based approach (Klar-Schmeiser, Lemou-Mieusseun) approach, we can also prove the following uniform stability:

$$\Delta t \le \frac{\sigma_{\min}}{3}\Delta x^2 + \frac{2\varepsilon}{3}\Delta x,$$

Numerical tests

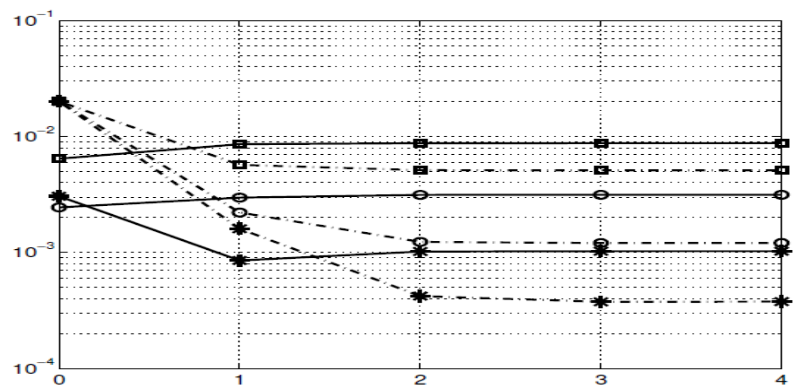


FIG. 8.13. *The linear transport equation: Errors of the mean (solid line) and standard deviation (dash line) of* $\overline{r}$ *(circle) with respect to the gPC order at* $\epsilon = 10^{-8}$*:* $\Delta x = 0.04$ *(squares),* $\Delta x = 0.02$ *(circles),* $\Delta = 0.01$ *(stars).*

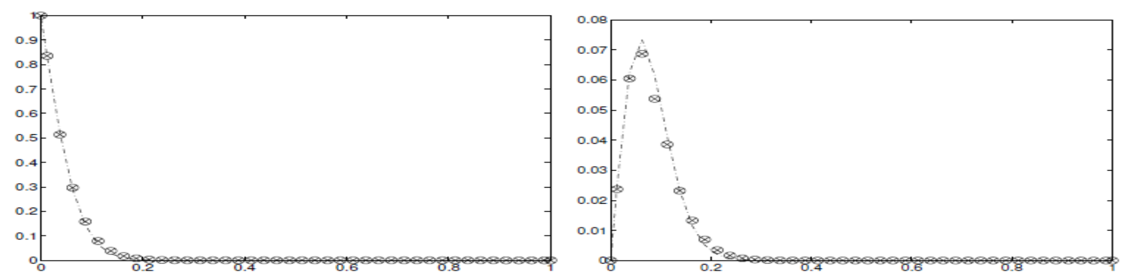


FIG. 8.14. *The linear transport equation: The mean (left) and standard deviation (right) of* $\overline{r}$ *at* $\epsilon = 10^{-8}$*, obtained by the gPC Galerkin at order* $N = 4$ *(circles), the stochastic collocation method (crosses), and the limiting analytical solution (8.6).*

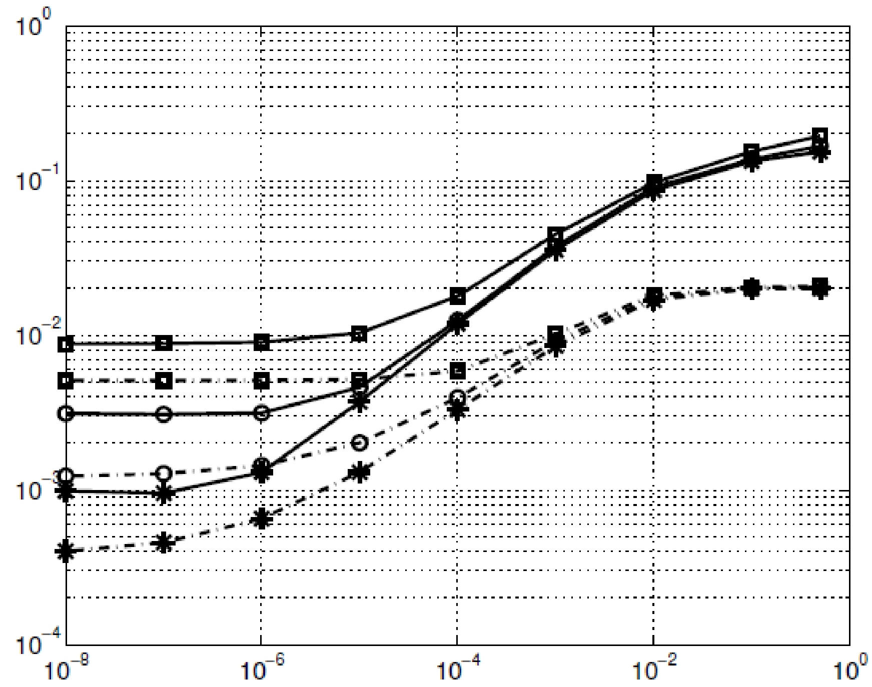


FIG. 8.15. *The linear transport equation: Differences in the mean (solid line) and standard deviation (dash line) of* $\overline{r}$ *with respect to* ϵ^2*, between the limiting analytical solution (8.6) and the 4th-order gPC solution with* $\Delta x = 0.04$ *(squares),* $\Delta x = 0.02$ *(circles) and* $\Delta x = 0.01$ *(stars).*

SG for the Boltzmann equation (J. Hu-J, JCP 2016)

The stochastic Boltzmann equation can be formulated as follows:

$$\begin{cases} \dfrac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}} f = \dfrac{1}{\varepsilon}\mathcal{Q}(f,f)(t,\mathbf{x},\mathbf{v},\mathbf{z}), & (0,t_{\max}]\times\Omega\times\mathbb{R}^d\times I_{\mathbf{z}}, \\ f(0,\mathbf{x},\mathbf{v},\mathbf{z}) = f^0(\mathbf{x},\mathbf{v},\mathbf{z}), & \Omega\times\mathbb{R}^d\times I_{\mathbf{z}}, \\ f(t,\mathbf{x},\mathbf{v},\mathbf{z}) = g(t,\mathbf{x},\mathbf{v},\mathbf{z}), & [0,t_{\max}]\times\partial\Omega\times\mathbb{R}^d\times I_{\mathbf{z}}, \end{cases}$$

where $\mathbf{z}$ is an n-**dimensional random vector** with support $I_{\mathbf{z}}$ characterizing the random inputs of the system. For simplicity, we assume $\mathbf{z}$ is a collection of random vectors $\mathbf{z}^B$, $\mathbf{z}^w$, $\mathbf{z}^i$ with mutually independent components

- collision kernel: $B = b_\lambda(\mathbf{z}^B)|\mathbf{v}-\mathbf{v}_*|^\lambda$
- boundary data: $T_w = T_w(t,\mathbf{x},\mathbf{z}^w)$, $\mathbf{u}_w = \mathbf{u}_w(t,\mathbf{x},\mathbf{z}^w)$
- initial data: $\rho^0(\mathbf{x},\mathbf{z}^i)$, $T^0(\mathbf{x},\mathbf{z}^i)$, $\mathbf{u}^0(\mathbf{x},\mathbf{z}^i)$

Stochastic Galerkin method

We seek a solution in the following form

$$f(t,\mathbf{x},\mathbf{v},\mathbf{z}) \approx P_K f = \sum_{|\mathbf{k}|=0}^{K} f_{\mathbf{k}}(t,\mathbf{x},\mathbf{v})\Phi_{\mathbf{k}}(\mathbf{z}),$$

$$f_{\mathbf{k}}(t,\mathbf{x},\mathbf{v}) = \frac{1}{\gamma_{\mathbf{k}}}\int_{I_z} f(t,\mathbf{x},\mathbf{v},\mathbf{z})\Phi_{\mathbf{k}}(\mathbf{z})\pi(\mathbf{z})\,d\mathbf{z}.$$

Here $\mathbf{k} = (k_1,\ldots,k_d)$ is a multi-index with $|\mathbf{k}| = k_1 + \cdots + k_d$. $\{\Phi_{\mathbf{k}}(\mathbf{z})\}$ are the gPC basis functions satisfying

$$\int_{I_z} \Phi_{\mathbf{k}}(\mathbf{z})\Phi_{\mathbf{j}}(\mathbf{z})\pi(\mathbf{z})\,d\mathbf{z} = \gamma_{\mathbf{k}}\delta_{\mathbf{kj}}, \quad 0 \le |\mathbf{k}|,|\mathbf{j}| \le K,$$

where $\pi(\mathbf{z})$ is the probability distribution function of $\mathbf{z}$, and $\gamma_{\mathbf{k}}$ are normalization factors. The above approximation is optimal in space $\mathbb{P}_K^d$ (the set of all d-variate polynomials of degree up to K) in the sense that

$$\|f - P_K f\|_{L^2_\pi} = \inf_{h\in\mathbb{P}_K^d} \|f-h\|_{L^2_\pi}.$$

Stochastic Galerkin method (cont'd)

Inserting the gPC expansion into the Boltzmann equation, and performing standard Galerkin projection, we get

$$\begin{cases} \dfrac{\partial f_{\mathbf{k}}}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_{\mathbf{k}} = \dfrac{1}{\varepsilon} Q_{\mathbf{k}}(t, \mathbf{x}, \mathbf{v}), \quad (0, t_{\max}] \times \Omega \times \mathbb{R}^d, \\ f_{\mathbf{k}}(0, \mathbf{x}, \mathbf{v}) = f_{\mathbf{k}}^0(\mathbf{x}, \mathbf{v}), \quad \Omega \times \mathbb{R}^d, \\ f_{\mathbf{k}}(t, \mathbf{x}, \mathbf{v}) = g_{\mathbf{k}}(t, \mathbf{x}, \mathbf{v}), \quad [0, t_{\max}] \times \partial\Omega \times \mathbb{R}^d, \end{cases}$$

for each $0 \le |\mathbf{k}| \le K$, and

$$Q_{\mathbf{k}} := \frac{1}{\gamma_{\mathbf{k}}} \int_{I_{\mathbf{z}}} \mathcal{Q}(P_K f, P_K f)(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \pi(\mathbf{z}) \, d\mathbf{z},$$

$$f_{\mathbf{k}}^0 := \frac{1}{\gamma_{\mathbf{k}}} \int_{I_{\mathbf{z}}} f^0(\mathbf{x}, \mathbf{v}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \pi(\mathbf{z}) \, d\mathbf{z},$$

$$g_{\mathbf{k}} := \frac{1}{\gamma_{\mathbf{k}}} \int_{I_{\mathbf{z}}} g(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \pi(\mathbf{z}) \, d\mathbf{z}.$$

Treatment of boundary condition

For the Maxwell boundary condition with uncertainty in the wall temperature T_w (assume $\mathbf{u}_w = 0$ for simplicity), $g_\mathbf{k}$ is given by

$$g_\mathbf{k} = (1-\alpha) f_\mathbf{k}(t, \mathbf{x}, \mathbf{v} - 2(\mathbf{v}\cdot n)n) + \alpha \sum_\mathbf{j} D_{\mathbf{kj}}(\mathbf{x}, \mathbf{v}) \int_{\mathbf{v}\cdot n<0} f_\mathbf{j}(t, \mathbf{x}, \mathbf{v}) |\mathbf{v}\cdot n| \, \mathrm{d}\mathbf{v}$$

where

$$D_{\mathbf{kj}}(\mathbf{x}, \mathbf{v}) := \frac{1}{\gamma_\mathbf{k}} \int_{I_\mathbf{z}} \frac{e^{-\frac{\mathbf{v}^2}{2T_w(\mathbf{x},\mathbf{z})}}}{(2\pi)^{\frac{d-1}{2}} T_w^{\frac{d+1}{2}}(\mathbf{x}, \mathbf{z})} \Phi_\mathbf{k}(\mathbf{z}) \Phi_\mathbf{j}(\mathbf{z}) \pi(\mathbf{z}) \, \mathrm{d}\mathbf{z}.$$

Treatment of collision term

For the VHS collision kernel with uncertainty in b_λ, $Q_{\mathbf{k}}$ can be further expanded as

$$Q_{\mathbf{k}} = \sum_{|\mathbf{i}|,|\mathbf{j}|=0}^{K} S_{\mathbf{kij}} \int_{\mathbb{R}^d} \int_{S^{d-1}} |\mathbf{v} - \mathbf{v}_*|^\lambda \left[f_{\mathbf{i}}(\mathbf{v}') f_{\mathbf{j}}(\mathbf{v}'_*) - f_{\mathbf{i}}(\mathbf{v}) f_{\mathbf{j}}(\mathbf{v}_*) \right] \mathrm{d}\sigma \mathrm{d}\mathbf{v}_*,$$

where

$$S_{\mathbf{kij}} := \frac{1}{\gamma_{\mathbf{k}}} \int_{I_{\mathbf{z}}} b_\lambda(\mathbf{z}) \Phi_{\mathbf{k}}(\mathbf{z}) \Phi_{\mathbf{i}}(\mathbf{z}) \Phi_{\mathbf{j}}(\mathbf{z}) \pi(\mathbf{z}) \, \mathrm{d}\mathbf{z}.$$

Note that $Q_{\mathbf{k}}$ still has 1, $\mathbf{v}$, $|\mathbf{v}|^2$ as collision invariants.

Evaluating $Q_{\mathbf{k}}$ is definitely the most expensive part. Can we do it efficiently?

Evaluating the collision operator — first reduction

$$Q_{\mathbf{k}} = \sum_{|\mathbf{i}|,|\mathbf{j}|=0}^{K} S_{\mathbf{kij}} \int_{\mathbb{R}^d} \int_{S^{d-1}} |\mathbf{v} - \mathbf{v}_*|^{\lambda} \left[f_{\mathbf{i}}(\mathbf{v}') f_{\mathbf{j}}(\mathbf{v}'_*) - f_{\mathbf{i}}(\mathbf{v}) f_{\mathbf{j}}(\mathbf{v}_*) \right] \mathrm{d}\sigma \mathrm{d}\mathbf{v}_*$$

For each fixed $\mathbf{k}$, decompose $S_{\mathbf{kij}}$ (via SVD) as

$$S_{\mathbf{kij}} = \sum_{r=1}^{R} U_{\mathbf{i}r}^{\mathbf{k}} V_{r\mathbf{j}}^{\mathbf{k}}, \quad R \le N_K = \dim(\mathbb{P}_K^d) = \binom{d+K}{d}$$

Substituting it into $Q_{\mathbf{k}}$ and rearranging terms, we get

$$Q_{\mathbf{k}} = \sum_{r=1}^{R} \int_{\mathbb{R}^d} \int_{S^{d-1}} |\mathbf{v} - \mathbf{v}_*|^{\lambda} \left[g_r^{\mathbf{k}}(\mathbf{v}') h_r^{\mathbf{k}}(\mathbf{v}'_*) - g_r^{\mathbf{k}}(\mathbf{v}) h_r^{\mathbf{k}}(\mathbf{v}_*) \right] \mathrm{d}\sigma \mathrm{d}\mathbf{v}_*$$

$$g_r^{\mathbf{k}}(\mathbf{v}) := \sum_{|\mathbf{i}|=0}^{K} U_{\mathbf{i}r}^{\mathbf{k}} f_{\mathbf{i}}(\mathbf{v}), \quad h_r^{\mathbf{k}}(\mathbf{v}) := \sum_{|\mathbf{i}|=0}^{K} V_{r\mathbf{i}}^{\mathbf{k}} f_{\mathbf{i}}(\mathbf{v}).$$

Evaluating the collision operator — second reduction

Note that

$$\begin{aligned} Q_{\mathbf{k}} &= \sum_{r=1}^{R} \int_{\mathbb{R}^d} \int_{S^{d-1}} |\mathbf{v} - \mathbf{v}_*|^{\lambda} \left[g_r^{\mathbf{k}}(\mathbf{v}') h_r^{\mathbf{k}}(\mathbf{v}'_*) - g_r^{\mathbf{k}}(\mathbf{v}) h_r^{\mathbf{k}}(\mathbf{v}_*) \right] \mathrm{d}\sigma \mathrm{d}\mathbf{v}_* \\ &= \sum_{r=1}^{R} \mathcal{Q}(g_r^{\mathbf{k}}, h_r^{\mathbf{k}}), \quad \mathcal{Q} \text{ is the original deterministic collision operator} \end{aligned}$$

One can apply the fast Fourier spectral method[1] in velocity space (with slight modification).

- Perthame-Pareschi
- Mouhot-Pareschi

Saved cost

$O(N_K^2 M^{d-1} N^d \log N)$ (compare with $O(N_K^3 N^{2d})$)

$N_K = 120$ if $K = 7, n = 3$, and $N_K = 792$ if $K = 7, n = 5$.

Boltzmann equation with random collision kernel

Assume $B(z) = 1 + sz$, $s = 0.6$, Knudsen number $\varepsilon = 0.1$.

$$f^0(x,v) = \frac{\rho^0(x)}{4\pi T^0(x)} \left(e^{-\frac{|v-u^0(x)|^2}{2T^0(x)}} + e^{-\frac{|v+u^0(x)|^2}{2T^0(x)}} \right), \quad x \in [0,1],$$

where

$$\rho^0(x) = \frac{2+\sin(2\pi x)}{3}, \quad u^0 = (0.2, 0), \quad T^0 = \frac{3+\cos(2\pi x)}{4}.$$

Boltzmann equation with random collision kernel

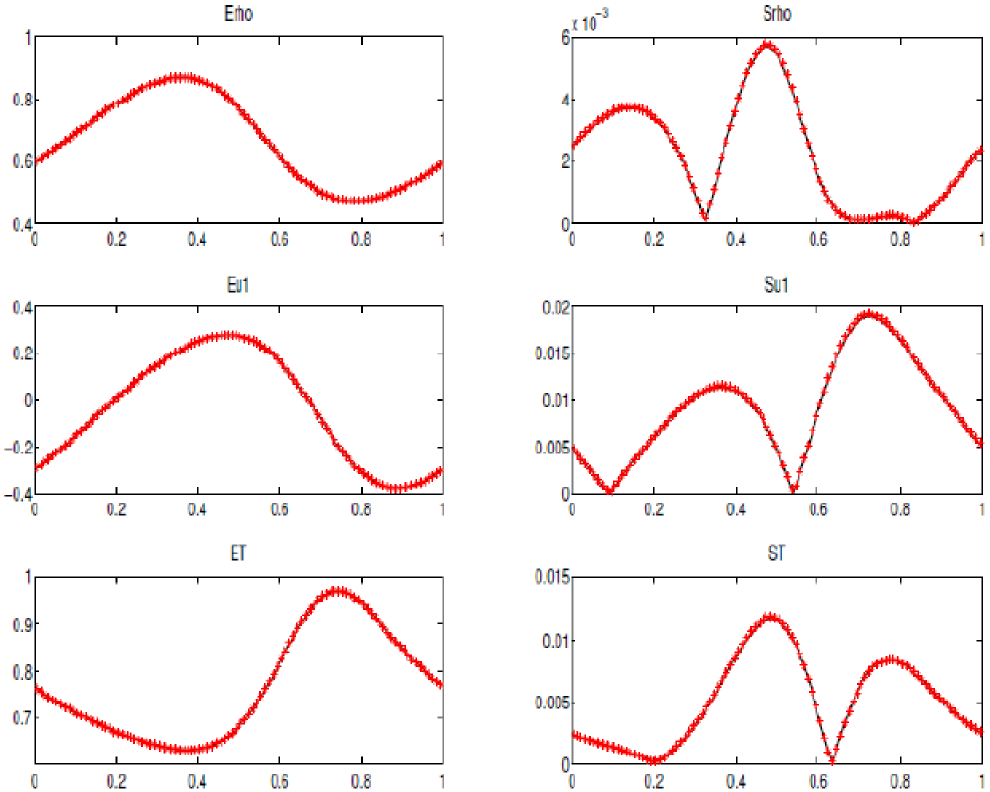


Figure: Solutions at $t = 0.2$. Solid line: collocation with $N_v = 64$, $M_v = 8$, $N_x = 200$, $N_z = 20$. Red star: Galerkin with $N_v = 32$, $M_v = 4$, $N_x = 100$, gPC mode: $K = 7$.

Boltzmann equation with random initial data

Consider continuous initial data

$$f^0(x,v) = \frac{\rho^0(x,z)}{4\pi T^0(x,z)} \left(e^{-\frac{|v-u^0(x)|^2}{2T^0(x,z)}} + e^{-\frac{|v+u^0(x)|^2}{2T^0(x,z)}} \right), \quad x \in [0,1],$$

where $u^0 = (0.2, 0)$, and

$$\rho^0(x,z) = \frac{2 + \sin(2\pi x) + \frac{1}{2}\sin(4\pi x) z_1 + \frac{1}{3}\sin(6\pi x) z_2}{3},$$

$$T^0(x,z) = \frac{3 + \cos(2\pi x) + \frac{1}{2}\cos(4\pi x) z_1 + \frac{1}{3}\cos(6\pi x) z_2}{4}.$$

Boltzmann equation with random initial data

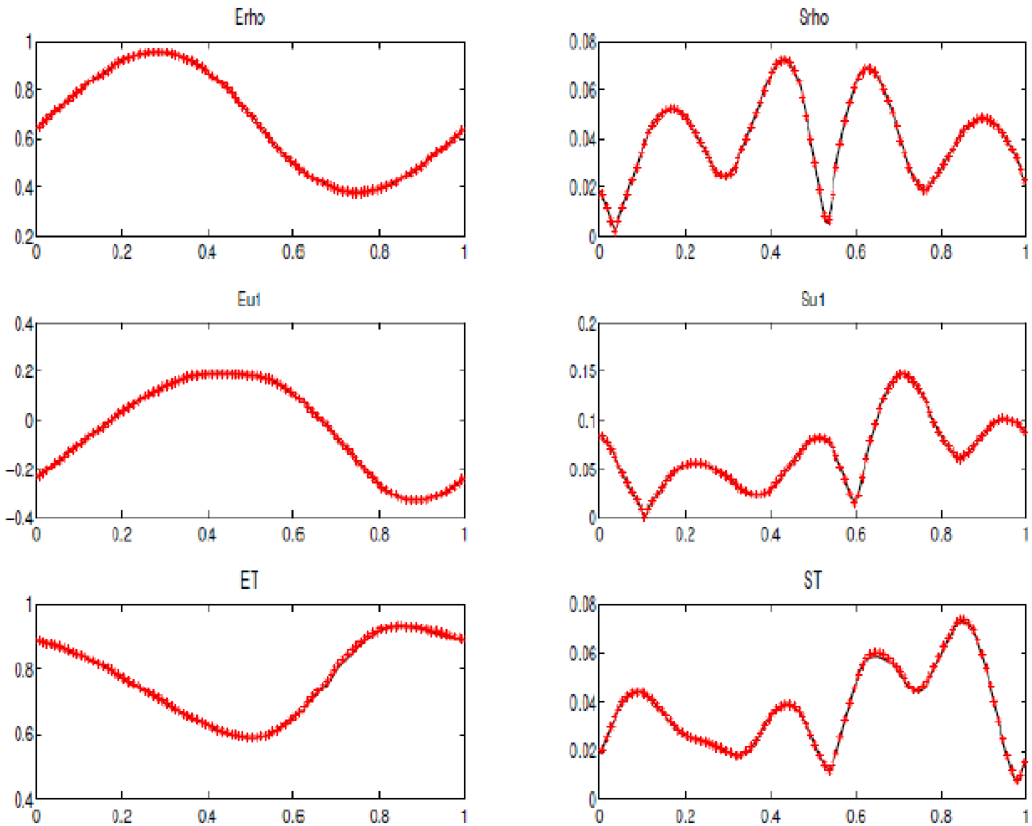


Figure: Solutions at $t = 0.1$. Solid line: collocation with $N_v = 64$, $M_v = 8$, $N_x = 200$, $N_z = 10$ (in each dimension). Red star: Galerkin with $N_v = 32$, $M_v = 4$, $N_x = 100$, gPC mode: $K = 5$.

Boltzmann equation with random boundary data

Consider **sudden heating problem**[2] (purely diffusive Maxwell boundary condition at left boundary $x = 0$).

$$f^0(x, v) = \frac{1}{2\pi T^0} e^{-\frac{v^2}{2T^0}}, \quad T^0 = 1, \quad x \in [0, 1].$$

At time $t = 0$, suddenly change the wall temperature to $T_w(z) = 2(T_0 + s_w z)$, $s_w = 0.2$, Knudsen number $\varepsilon = 0.1$.

[2] Aoki et al., 1991.

Boltzmann equation with random boundary data

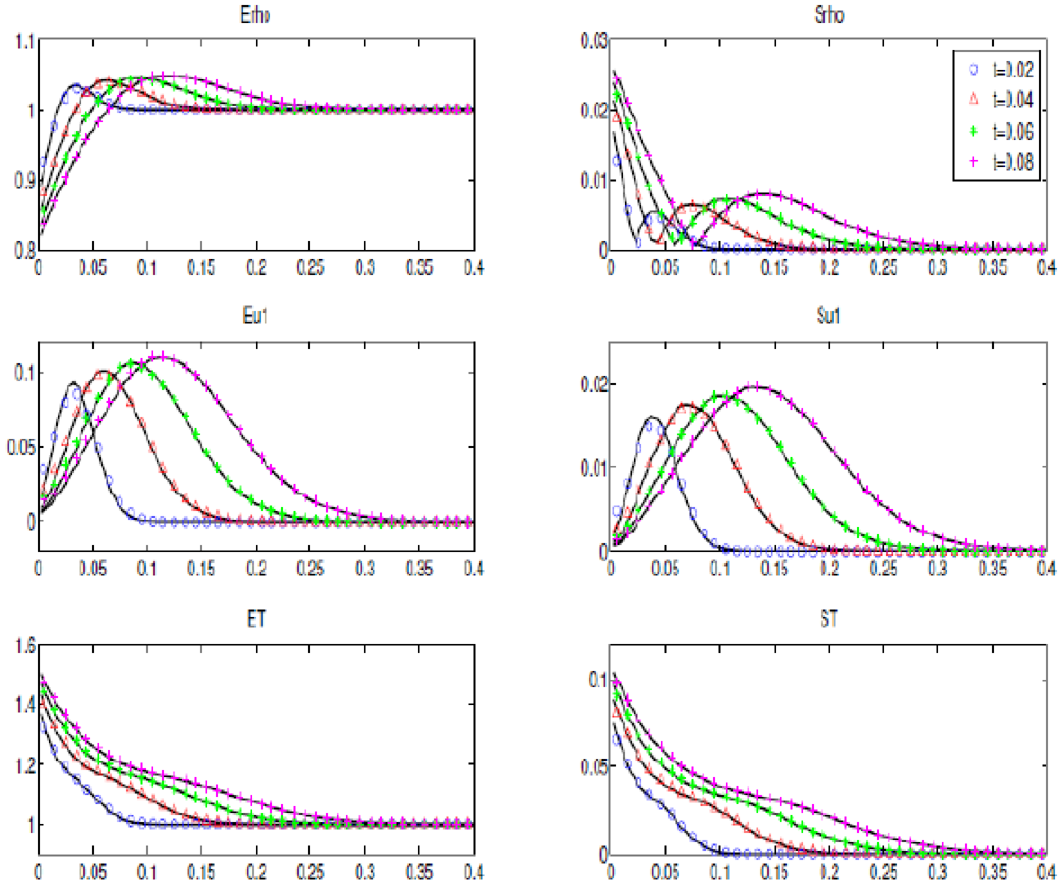


Figure: Solutions at $t = 0.1$. Solid line: collocation with $N_v = 64$, $M_v = 8$, $N_x = 200$, $N_z = 20$. Galerkin with $N_v = 32$, $M_v = 4$, $N_x = 100$, $K = 7$.

A kinetic-fluid disperse two-phase flow model

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla_x \Phi \cdot \nabla_v f = \mathcal{L}_u f, \\ \partial_t u + \nabla_x \cdot (u \otimes u) + \nabla_x p - \dfrac{1}{Re} \Delta_x u = \kappa \displaystyle\int (v-u) f \, \mathrm{d}v, \\ \nabla_x \cdot u = 0, \end{cases}$$

- u : velocity field of the primary phase
- f : particle distribution of the secondary phase
- $\mathcal{L}_u f = \nabla_v \cdot ((v-u)f + \nabla_v f).$ Fokker-Planck operator

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Goudon-Jabin-Vasseur (2004)

conservation property, energy-entropy dissipation

- Mass conservation: $\frac{\mathrm{d}}{\mathrm{d}t}\int \langle f \rangle \mathrm{d}x = 0$
- Momentum conservation: $\frac{\mathrm{d}}{\mathrm{d}t}\int (u + \langle v f \rangle)\mathrm{d}x = 0$
- Energy-entropy dissipation

$$\frac{\mathrm{d}}{\mathrm{d}t}\int \left(\frac{|u|^2}{2} + \langle f \ln f + \frac{|v|^2}{2} f \rangle \right) \mathrm{d}x \leq 0$$

Fine particle scaling

$$\begin{cases} \partial_t f + v \cdot \nabla_x f - \nabla_x \Phi \cdot \nabla_v f = \frac{1}{\epsilon} \mathcal{L}_u f, \\ \partial_t u + \nabla_x \cdot (u \otimes u) + \nabla_x p - \frac{1}{Re} \Delta_x u = \frac{1}{\epsilon} \kappa \int (v - u) f \, \mathrm{d}v, \\ \nabla_x \cdot u = 0. \end{cases}$$

$$\epsilon \to 0 \quad \longrightarrow \quad \mathcal{L}_u f = 0 \quad \longrightarrow \quad \boxed{\begin{aligned} &f(t,x,v) = n(t,x) M_u(v), \\ &M_u(v) = \frac{1}{(2\pi)^{d_v/2}} \exp\left(-\frac{|v-u(t,x)|^2}{2}\right), \end{aligned}}$$

$$\mathcal{L}_u f = \nabla_v \cdot ((v-u) f + \nabla_v f).$$

$$n(t,x) = \int f(t,x,v) \, \mathrm{d}v, \quad J(t,x) = \int v f(t,x,v) \, \mathrm{d}v, \quad P(t,x) = \int v \otimes v f(t,x,v) \, \mathrm{d}v.$$

Hydrodynamic limit

$$J = nu, \quad P = nu \otimes u + nI,$$

$$\begin{cases} \partial_t n + \nabla_x \cdot (nu) = 0, \\ \partial_t((1+\kappa n)u) + \nabla_x((1+\kappa n)u \otimes u) + \nabla_x(p + \kappa n) + \kappa n \nabla_x \Phi = \dfrac{1}{Re}\Delta_x u, \end{cases}$$

variable density incompressible Navier-Stokes equations

gPC- SG for two-phase flow (J-R. Shu, JCP '17)

- Considering uncertainty from initial data (can also come from other sources: Y. Zhu-J MMS '17)

$$\begin{cases} \partial_t \vec{f} + v \cdot \nabla_x \vec{f} - \nabla_x \Phi \cdot \nabla_v \vec{f} = \frac{1}{\epsilon} \vec{\mathcal{L}}_{\vec{u}} \vec{f}, \\ \partial_t \vec{u}^{(i)} + \partial_{x_1} (A^{(i)} \vec{u}^{(1)}) + \partial_{x_2} (A^{(i)} \vec{u}^{(2)}) + \partial_{x_i} \vec{p} - \frac{1}{Re} \Delta_x \vec{u}^{(i)} = \frac{1}{\epsilon} \kappa \int (v_i - A^{(i)}) \vec{f} \, \mathrm{d}v, \quad i = 1, 2, \\ \nabla_x \cdot \vec{u} = 0, \end{cases}$$

$$S_{ijk} = \int \phi_i \phi_j \phi_k \pi(z) \, \mathrm{d}z.$$

- Vector notation $\vec{g} = (g_1, \dots, g_K)^T$
- Multiplication by g(z) becomes $A(g)_{ij} = \sum_{k=1}^{K} S_{ijk} g_k \qquad A^{(1)} = A(u^{(1)})$
- Vectorized Fokker-Planck operator

$$\vec{\mathcal{L}}_{\vec{u}}(\vec{f}) = \Delta_v \vec{f} + \partial_{v_1}(v_1 \vec{f}) + \partial_{v_2}(v_2 \vec{f}) - \partial_{v_1}(A^{(1)} \vec{f}) - \partial_{v_2}(A^{(2)} \vec{f}),$$

sAP property

$$\vec{\mathcal{L}}_{\vec{u}}(\vec{f}) = \Delta_v \vec{f} + \partial_{v_1}(v_1 \vec{f}) + \partial_{v_2}(v_2 \vec{f}) - \partial_{v_1}(A^{(1)} \vec{f}) - \partial_{v_2}(A^{(2)} \vec{f}),$$

- Vectorized FP operator is weakly nonlinear: $A^{(1)}, A^{(2)}$ are constant symmetric matrices if u is fixed, but they do not commute in general.
- Theorem: $\boxed{\vec{\mathcal{L}}_{\vec{u}} = \vec{\mathcal{T}}_{\vec{u}} \vec{\mathcal{L}}_{\vec{0}} \vec{\mathcal{T}}_{\vec{u}}^{-1}.}$

$$\vec{\mathcal{T}}_{\vec{u}}(\vec{f}) = \exp(-A^{(1)}\partial_{v_1} - A^{(2)}\partial_{v_2})(\vec{f}).$$

- Null space of $\vec{\mathcal{L}}_{\vec{u}}$: $\vec{M}(v) = \vec{\mathcal{T}}_{\vec{u}}(M_0 \vec{C})$
- $M_0 = \frac{1}{2\pi} \exp(-\frac{|v|^2}{2})$ $\vec{C}$ is any constant vector

- Hydrodynamic limit of gPC-sG system:

$$
\begin{cases}
\partial_t \vec{n} + \nabla_x \cdot (A\vec{n}) = 0, \\
\partial_t (\vec{u}^{(i)} + \kappa A^{(i)} \vec{n}) + \nabla_x \cdot [A\vec{u}^{(i)} + \frac{\kappa}{2}(A^{(i)}A + AA^{(i)})\vec{n}] \\
\qquad\qquad + \partial_{x_i}(\vec{p} + \kappa \vec{n}) + \kappa \vec{n} \partial_{x_i} \Phi = \frac{1}{Re} \Delta_x \vec{u}^{(i)}, \quad i = 1, 2.
\end{cases}
$$

is the gPC-sG system for the limiting NS equations

S-AP

Treat $\vec{\mathcal{L}}_{\vec{u}}$ implicitly

- In order to achieve AP for the time discretization, one needs to treat the stiff operator $\vec{\mathcal{L}}_{\vec{u}} = \vec{\mathcal{T}}_{\vec{u}}\vec{\mathcal{L}}_{\vec{0}}\vec{\mathcal{T}}_{\vec{u}}^{-1}$. implicitly.

- A direct computation of $\vec{\mathcal{T}}_{\vec{u}}(\vec{f}) = \exp(-A^{(1)}\partial_{v_1} - A^{(2)}\partial_{v_2})(\vec{f})$. using Fourier transform will require N_v^2 times of matrix exponential of size K.

- Using a spectrally accurate splitting

$$\exp(-A^{(1)}\partial_{v_1} - A^{(2)}\partial_{v_2})\vec{f} \approx \exp(-A^{(1)}\partial_{v_1})\exp(-A^{(2)}\partial_{v_2})\vec{f}.$$

we reduce the number of matrix exponentials to 2.

Numerical results

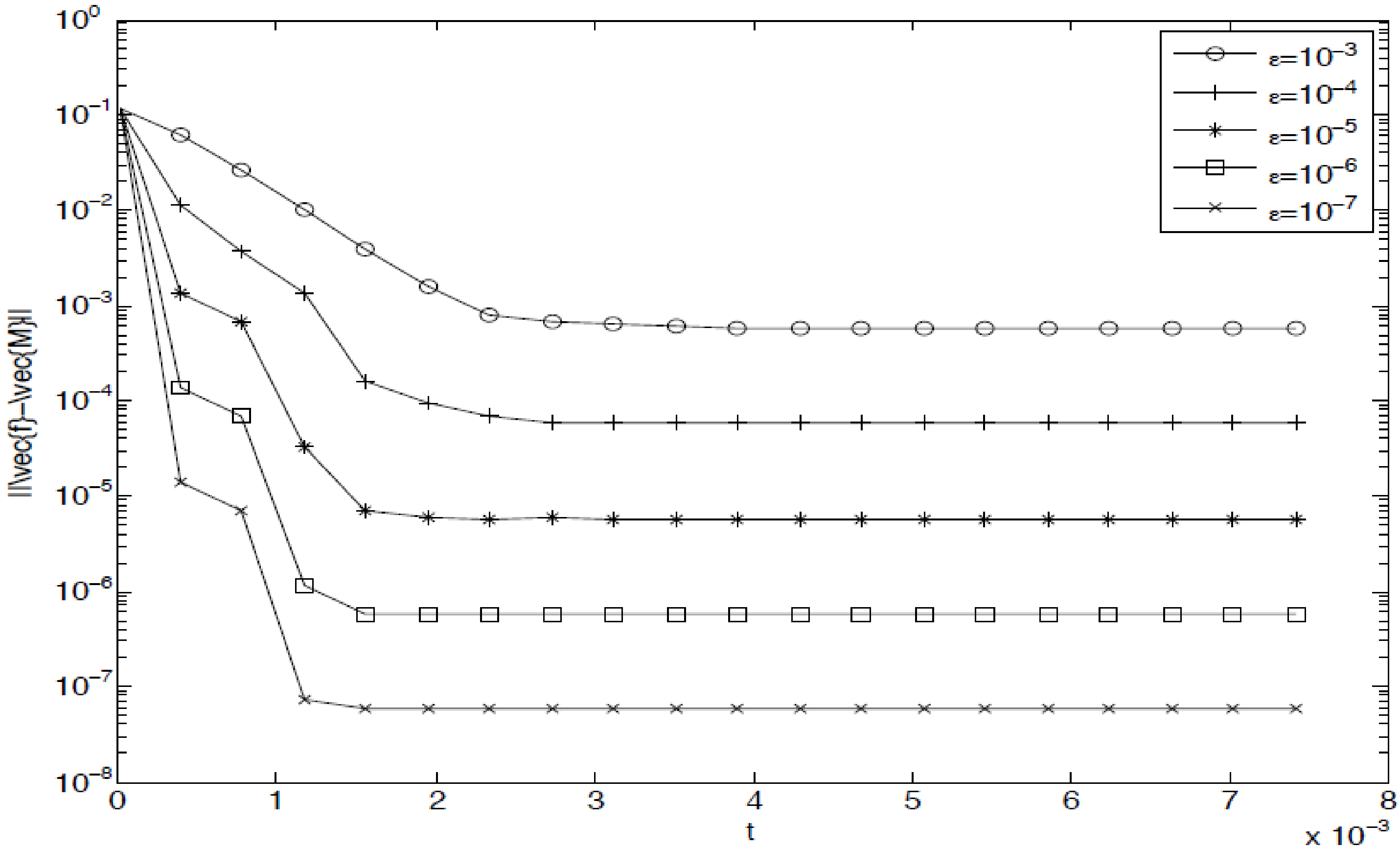
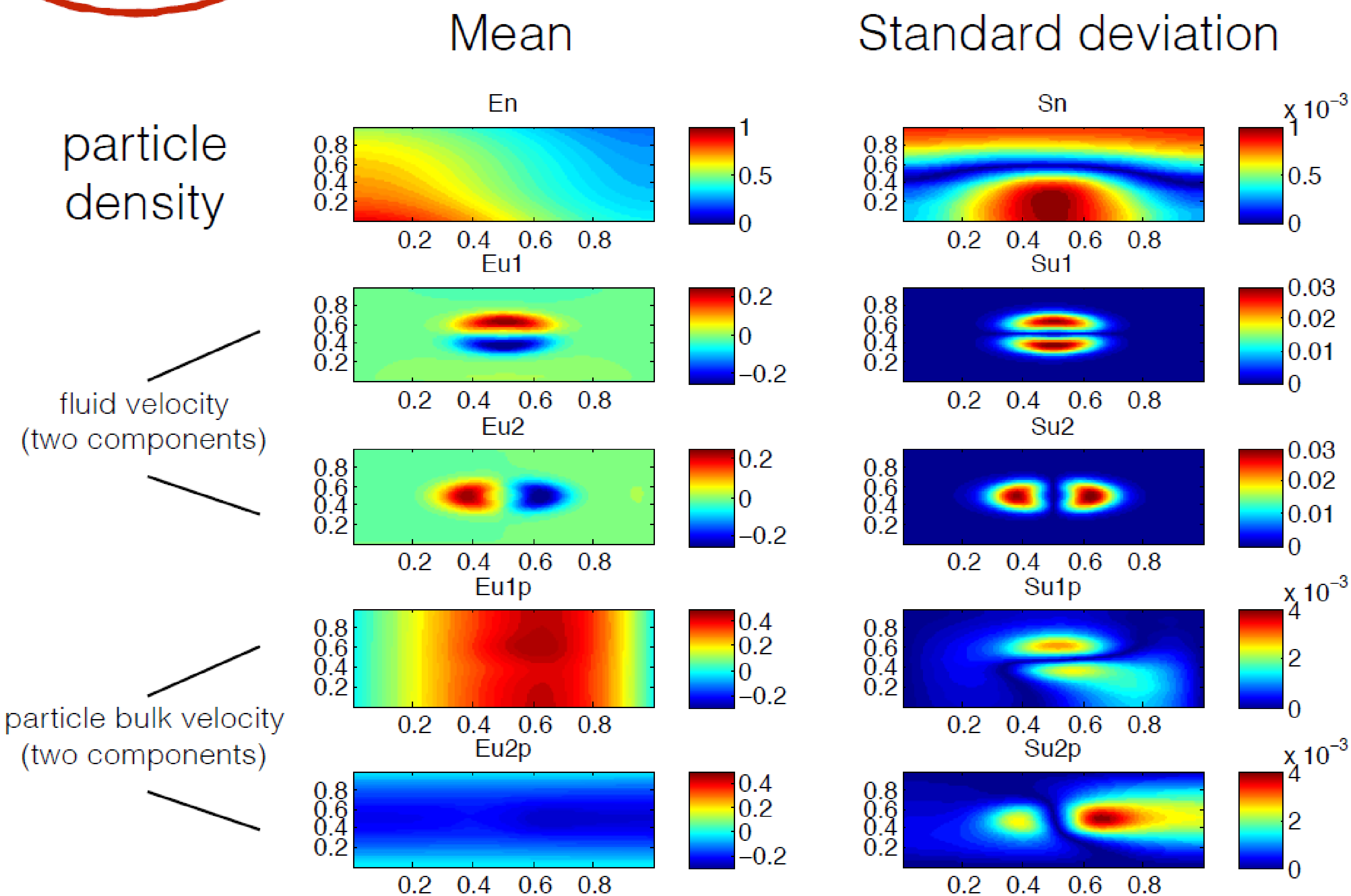


Figure 1: The s-AP property: time evolution of $\|\vec{f} - \vec{M}\|$ measured in $L^\infty_x(L^2_{v,z})$, $\epsilon = 10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}$.

$\epsilon = 1$



Mean
Standard deviation
particle density
fluid velocity
(two components)
particle bulk velocity
(two components)
En
Sn
x 10^-3
Eu1
Su1
Eu2
Su2
Eu1p
Su1p
Eu2p
Su2p

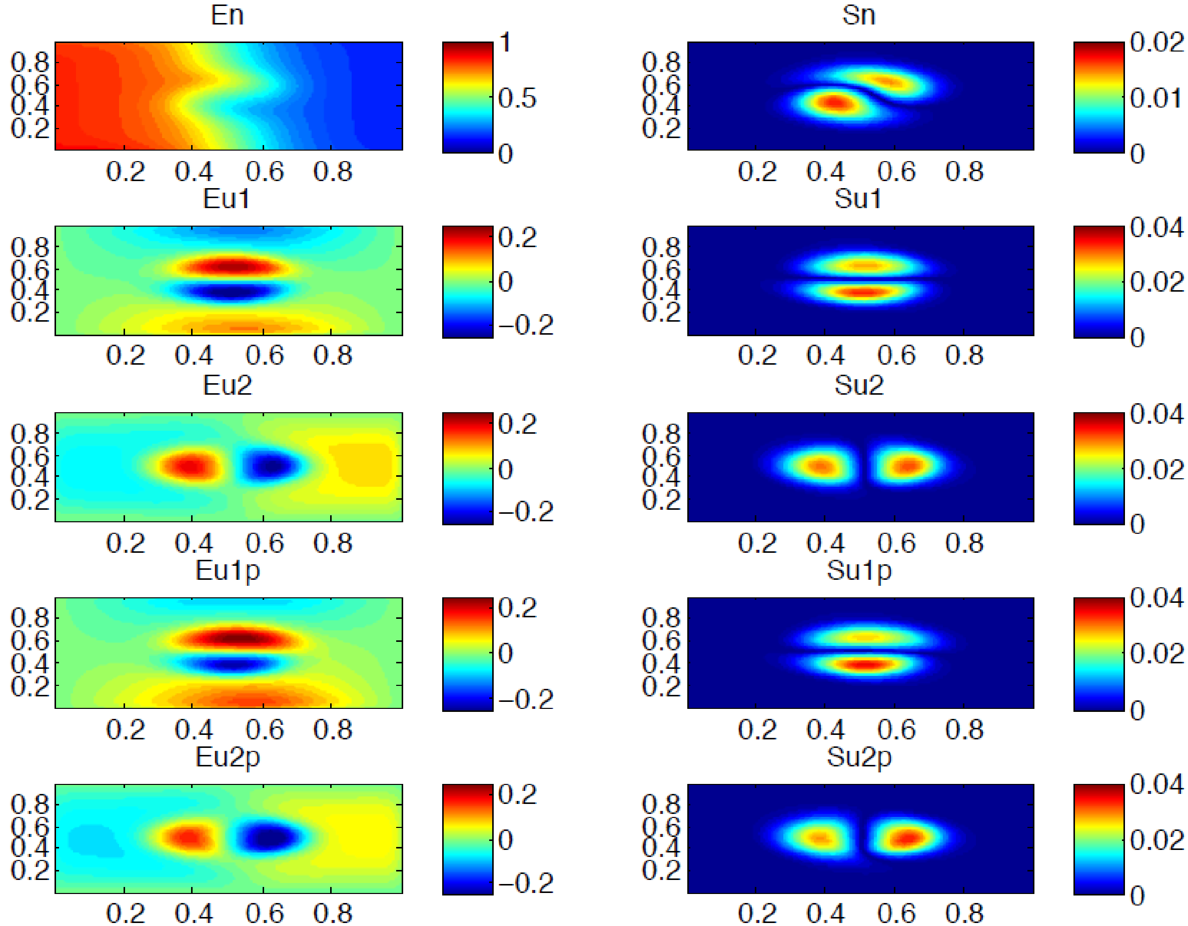
$\epsilon = 0.01$

	Mean	Standard deviation

particle density

fluid velocity (two components)

particle bulk velocity (two components)



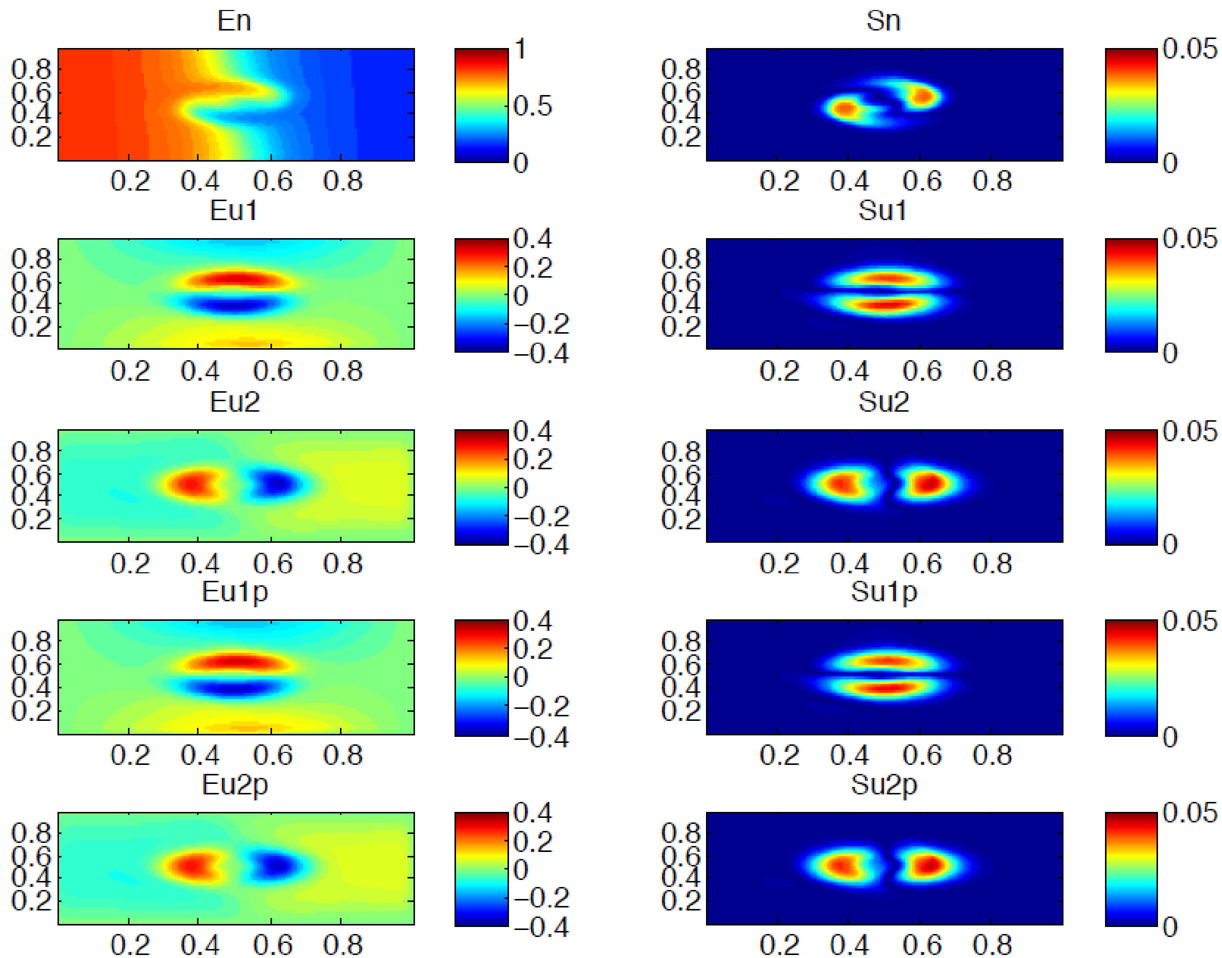
$\epsilon = 10^{-8}$

Mean   Standard deviation

particle density

fluid velocity (two components)

particle bulk velocity (two components)



gPC-SG for many different kinetic equations

- Boltzmann: a fast algorithm for collision operator (J. Hu-Jin, JCP '16), initial regularity in the random space is preserved in time; but not clear whether it is unifornly stable in the fluid dynamics limit (s-AP?): gPC-SG for nonlinear hyperbolic system is not globally hpperbolic! (APUQ is open)
- Landau equation (J. Hu-Jin-R. Shu, '17):
- Semiconductor Boltzmann-drift diffusion limit (uniform regularity. Jin-L. Liu MMS 17, Uniform spectral convergence : L. Liu '17)
- Radiative heat transfer (APUQ OK: Jin-H. Lu JCP'17): proof of regularity in random space for linearized problem (nonlinear? Open)
- Kinetic-incompresssible fluid couple models for disperse two phase flow: (efficient algorithm in multi-D: Jin-Shu)