Uncertainty Quantification for multiscale kinetic equations with high dimensional random inputs with sparse grids

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Kinetic equations

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon} \mathcal{Q}(f, f)(\mathbf{v}), \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \ \mathbf{v} \in \mathbb{R}^d$$

- $f(t, \mathbf{x}, \mathbf{v})$ is the **phase space distribution function** of time t, position $\mathbf{x}$, and velocity $\mathbf{v}$
- ε is the **Knudsen number**, ratio of the mean free path and the characteristic length scale: $\varepsilon \sim O(1)$ kinetic regime; $\varepsilon \ll O(1)$ fluid regime
- $\mathcal{Q}(f, f)$ is the **collision operator**, a quadratic integral operator modeling the interaction of particles

Different Q

- Boltmann
- Landau for collisional plasma
- Fokker-Planck
- Neutron transport
- Radiative transfer
- Semiconductor Boltzmann
- Quantum Boltzmann
- etc

Major challenges

- Multiscale
- Random inputs
- Dimensional curse (6 dimension + dimension of random variables)

Scales in kinetic equations

- When ε is small ($kn \leq 0.01$), the moments of f solve the compressive Euler (to leading order) or Navier-Stokes equations (to $O(\varepsilon)$) of fluid dynamics, except at initial, boundary or shock layers
- When ε is not small the fluid equations are not valid, so one has to use the kinetic equations

Other scales

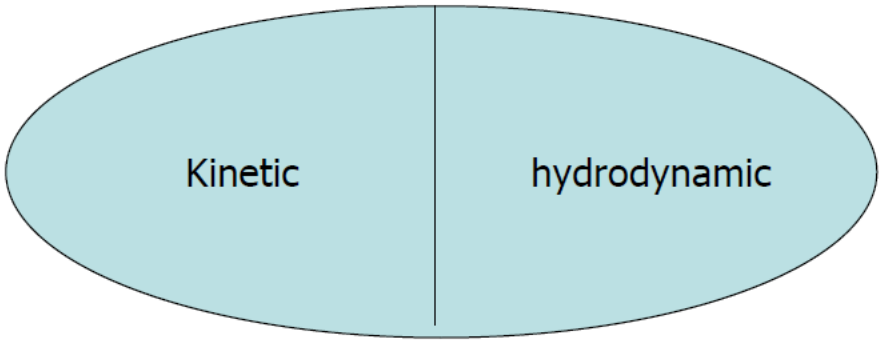
- High field limit (balance of collision with strong electric/magnetic field)
- Quasineutral limit
- Incompressible Euler/Navier-Stokes or diffusion limit

- etc.

A typical multi-physics/multiscale approach

- Domain decomposition methods are useful in multiscale computation:

  coupling of microscopic and macroscopic models: multiphysics simulation



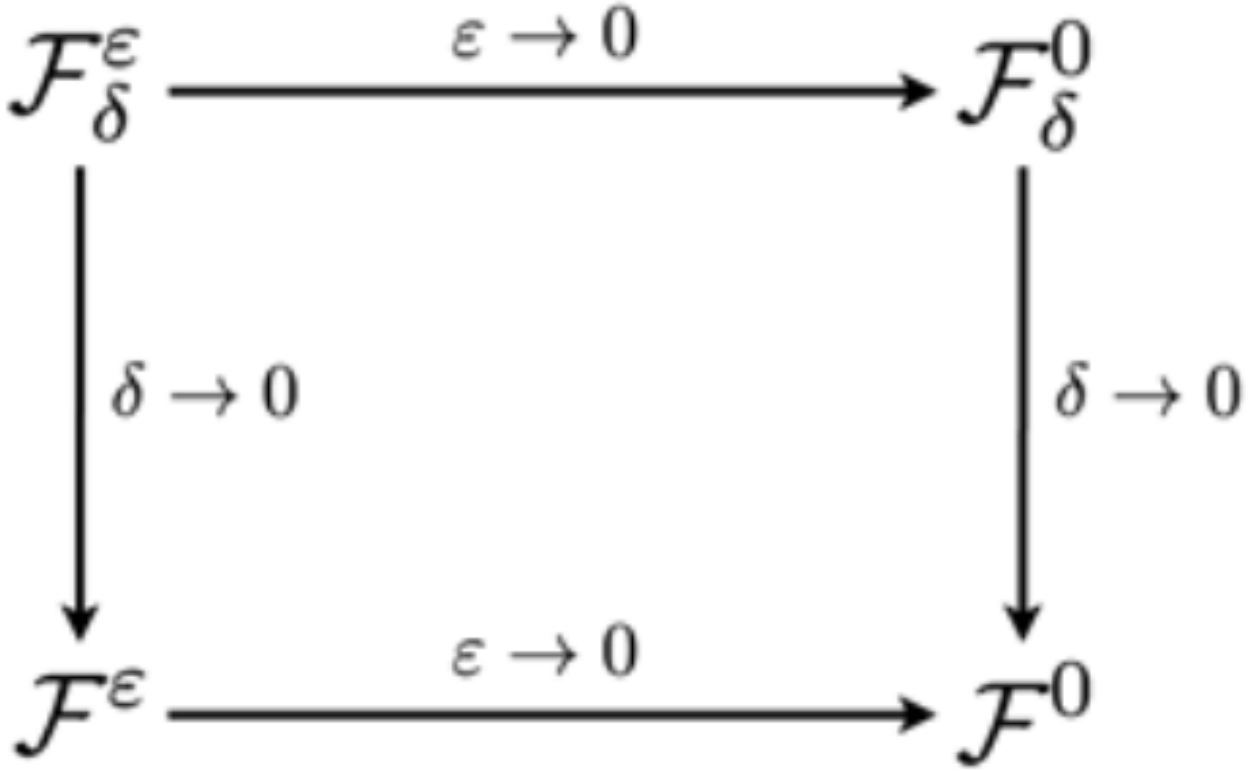
The difficulty is the interface condition: how to transfer data between different scales—often no unique solution; where to put the interface?

Asymptotic-preserving (AP) method -- a different multiscale paradigm

- Work in both kinetic and fluid regimes

  by solving only the kinetic equation
- When ε is small, and $\Delta x, \Delta t >> \varepsilon$ they automatically become a fluid dynamic solver
- No coupling with macroscopic equations, thus avoid the difficulty of interface condition/treatment as in other multiscale methods

AP diagram (Jin ‘99)



Developments of AP schemes

- Since the 90s there have been many developments of AP schemes for various kinetic and hyperbolic equations:

  time-independent: Larsen-Morel-Miller '89, Jin-Levermore '93,

  time-dependent: Jin '99, Jin-Pareschi-Toscani '99, Klar '99, Degond etc '05, Lemou-Mieusseun '08, Filbet-Jin '11, Xu etc. '15, …

- Reviews

  Jin '12, Acta Numerica (general), Degond '13 (for plasma) and Degond-Deluzet 16, JCP (for Plasma)

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
- While UQ has been popular in solid mechanics, CFD, elliptic equations, etc. there has been little effort for kinetic equation

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

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

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).

Intrusive vs Non-Intrusive

- Intrusive: stochastic Galerkin, change the equations and solvers, nice mathematical formulation, better accuracy,
- Non-intrusive stochastic collocation methods: running deterministic solvers, for samplings chosen to be the zeroes of the orthogonal polynomials rather than the Monte-Carlo samplings; using interpolations/quadrature rules to get information at non-sampling points and other quantities of interests
- Higher dimension using sparse grids

- Babuska, Ghanem-Spanos, Gunzburger, Hesthaven, Hou, Karniadakis, Knio, Le Maitre, Majda, Mishira, Oden, Schwab, Stuart, Tempone, Webster, Xiu, …

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.*

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

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

Rigorous analysis (J-J.G. Liu-Z. Ma)

- The regularity in the random space is preserved in time, uniformly in ε

$$D^k f(t,x,v,z) := \partial_z^k f(t,x,v,z)$$

Theorem 4.1 (Uniform regularity). *Assume*

$$\sigma(z) \geq \sigma_{\min} > 0\,.$$

If for some integer $m \geq 0$,

$$\|D^k \sigma(z)\|_{L^\infty} \leq C_\sigma, \qquad \|D^k f_0\|_{\Gamma(0)} \leq C_0, \qquad k = 0, \ldots, m,$$

then

$$\|D^k f\|_{\Gamma(t)} \leq C, \qquad k = 0, \cdots, m, \qquad \forall t > 0,$$

where C_σ, C_0 *and* C *are constants independent of* ε.

- A good problem to use the gPC-SG for UQ

Uniform spectral accuracy

- Define the following norms

$$\langle f, g\rangle_\omega = \int_{\mathbb{R}^d} f(z)g(z)\,\omega(z)\,\mathrm{d}z, \quad \|f\|_\omega^2 = \langle f, f\rangle_\omega$$

$$\|f(t,x,v,\cdot)\|_{H^k}^2 := \sum_{\alpha\le k} \|D^\alpha f(t,x,v,\cdot)\|_\omega^2$$

$$\|f(t,\cdot,\cdot,\cdot)\|_{\Gamma(t)}^2 := \int_Q \|f(t,x,v,\cdot)\|_\omega^2 \,\mathrm{d}x\,\mathrm{d}v,$$

- Then

Theorem 4.3 (Uniformly convergence in ε). *Assume*

$$\sigma(z) \ge \sigma_{\min} > 0\,.$$

If for some integer $m \ge 0$,

$$\|\sigma(z)\|_{H^k} \le C_\sigma, \quad \|D^k f_0\|_{\Gamma(0)} \le C_0, \quad \|D^k(\partial_x f_0)\|_\omega \le C_x, \quad k = 0,\dots,m, \tag{82}$$

Then the error of the whole gPC-SG method is

$$\|f - f_N\|_{\Gamma(t)} \le \frac{C(T)}{N^k}, \tag{83}$$

where $C(T)$ is a constant independent of ε.

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:

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

Numerical tests

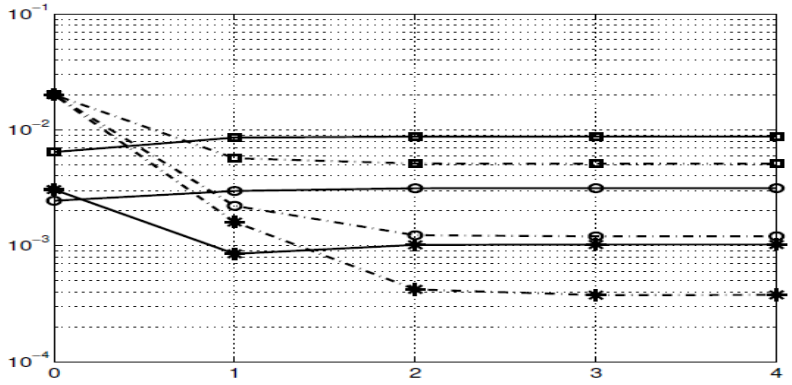


FIG. 8.13. *The linear transport equation: Errors of the mean (solid line) and standard deviation (dash line) of $\overline{r}$ (circle) with respect to the gPC order at $\epsilon = 10^{-8}$: $\Delta x = 0.04$ (squares), $\Delta x = 0.02$ (circles), $\Delta = 0.01$ (stars).*

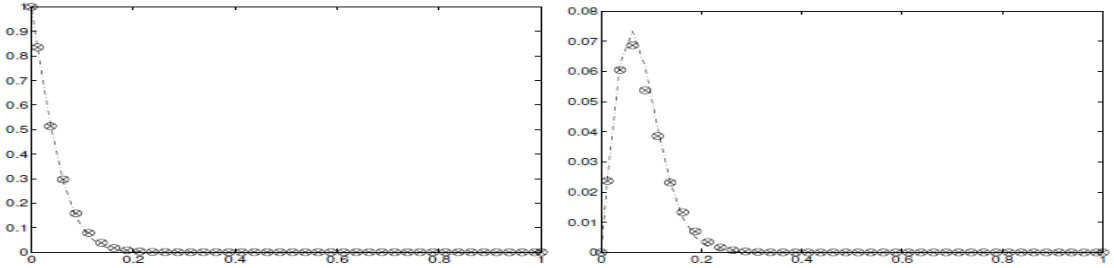


FIG. 8.14. *The linear transport equation: The mean (left) and standard deviation (right) of $\overline{r}$ at $\epsilon = 10^{-8}$, obtained by the gPC Galerkin at order $N = 4$ (circles), the stochastic collocation method (crosses), and the limiting analytical solution* (8.6).

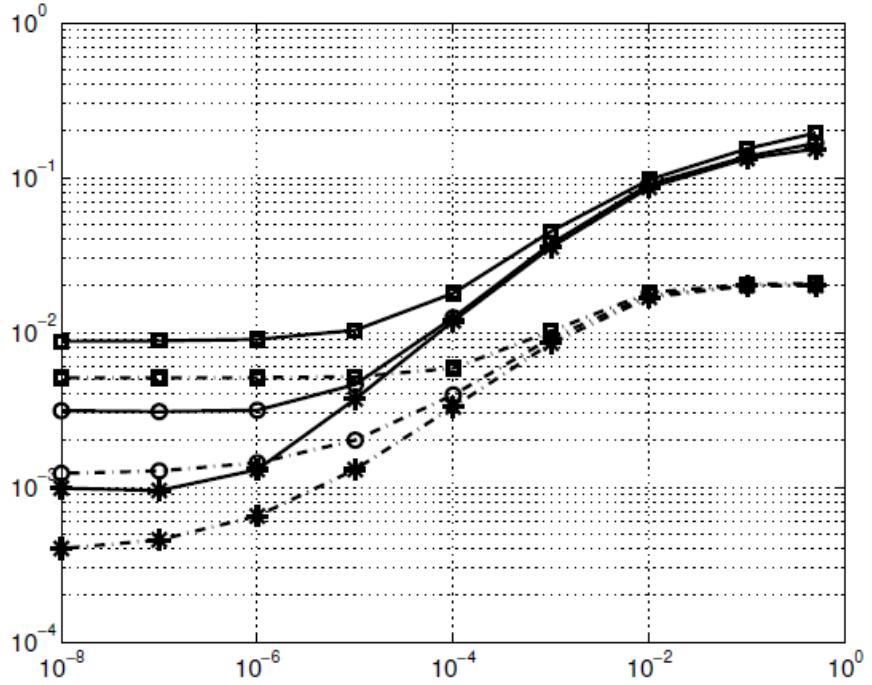


FIG. 8.15. *The linear transport equation: Differences in the mean (solid line) and standard deviation (dash line) of* $\overline{r}$ *with respect to* ϵ^2*, between the limiting analytical solution* (8.6) *and the 4th-order gPC solution with* $\Delta x = 0.04$ *(squares),* $\Delta x = 0.02$ *(circles)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

Boltzmann equation with high dimensional random inputs (with Ruiwen Shu, Jingwei Hu)

time space velocity

- $\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = Q(f, f), \quad t \in \mathbb{R}^+, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^{d_x}, \ \mathbf{v} \in \mathbb{R}^{d_v}$
- $f = f(t, \mathbf{x}, \mathbf{v})$: distribution function of particles
- Collision operator: $Q(f, g) = \int_{\mathbb{R}^d} \int_{\mathbb{S}^{d-1}} B(\mathbf{v}, \mathbf{v}_*, \sigma)(f(\mathbf{v}')g(\mathbf{v}'_*) - f(\mathbf{v})g(\mathbf{v}_*))\mathrm{d}\sigma\mathrm{d}\mathbf{v}_*$
- Collision kernel: $B(\mathbf{v}, \mathbf{v}_*, \sigma) = B(|v - v_*|, \cos\theta), \quad \cos\theta = \frac{\sigma \cdot (\mathbf{v} - \mathbf{v}_*)}{|\mathbf{v} - \mathbf{v}_*|}$
- Pre/post collision velocity $\begin{cases} \mathbf{v}' = \dfrac{\mathbf{v} + \mathbf{v}_*}{2} + \dfrac{|\mathbf{v} - \mathbf{v}_*|}{2}\sigma, \\ \mathbf{v}'_* = \dfrac{\mathbf{v} + \mathbf{v}_*}{2} - \dfrac{|\mathbf{v} - \mathbf{v}_*|}{2}\sigma. \end{cases}$

Properties of $Q(f,g)$

- Conservation: $\int_{\mathbb{R}^d} Q(f,f)(1,\mathbf{v},|\mathbf{v}|^2)^T \mathrm{d}\mathbf{v} = 0$
- H-theorem: $\int_{\mathbb{R}^d} Q(f,f)\log f \mathrm{d}\mathbf{v} \leq 0$
- Local equilibrium: $M(\mathbf{v}) = \dfrac{\rho}{(2\pi T)^{d/2}} \exp(-\dfrac{|\mathbf{v}-\mathbf{u}|^2}{2T})$
- ρ : density, $\mathbf{u}$: velocity, T : temperature

$$\rho = \int f \mathrm{d}\mathbf{v}, \quad \mathbf{u} = \frac{1}{\rho}\int f\mathbf{v}\mathrm{d}\mathbf{v}, \quad T = \frac{1}{d\rho}\int f|\mathbf{v}-\mathbf{u}|^2\mathrm{d}\mathbf{v}$$

Boundary Condition

- Maxwell boundary condition

$$f(t,\mathbf{x},\mathbf{v}) = g(t,\mathbf{x},\mathbf{v}), \quad \mathbf{x}\in\partial\Omega, \quad \mathbf{v}\cdot\mathbf{n}>0,$$

$$g(t,\mathbf{x},\mathbf{v}) = (1-\alpha) f(t,\mathbf{x},\mathbf{v}-2(\mathbf{v}\cdot\mathbf{n})\mathbf{n})$$

$$+ \frac{\alpha}{(2\pi)^{(d_v-1)/2} T_w^{(d_v+1)/2}} e^{-\frac{|\mathbf{v}|^2}{2T_w}} \int_{\mathbf{v}\cdot\mathbf{n}<0} f(t,\mathbf{x},\mathbf{v})|\mathbf{v}\cdot\mathbf{n}|\mathrm{d}\mathbf{v}$$

reflective

diffusive

- T_w : wall temperature, α : accommodation coefficient

BE with uncertainty [1]

$$\partial_t f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) = Q_{\mathbf{z}}(f, f)$$
$$t \in \mathbb{R}_+, \mathbf{x} \in \Omega, \mathbf{v} \in \mathbb{R}^{d_v}, \mathbf{z} \in I_{\mathbf{z}}$$

- $\mathbf{z}$: random variable
- $I_{\mathbf{z}}$: d-dimensional random space, with probability distribution $\pi(\mathbf{z})$
- Random collision kernel: $B(\mathbf{v}, \mathbf{v}_*, \omega, \mathbf{z}) = b(\mathbf{z}) B_0(\mathbf{v}, \mathbf{v}_*, \omega)$
- Random boundary condition: $T_w(\mathbf{z}), \alpha(\mathbf{z})$

SG Method for BE

$$\partial_t f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) + \mathbf{v} \cdot \nabla_{\mathbf{x}} f(t, \mathbf{x}, \mathbf{v}, \mathbf{z}) = Q_{\mathbf{z}}(f, f)$$

$$\partial_t \hat{f}_k(t, \mathbf{x}, \mathbf{v}) + \mathbf{v} \cdot \nabla_{\mathbf{x}} \hat{f}_k(t, \mathbf{x}, \mathbf{v}) = Q_k(f^K, f^K), \quad k = 0, 1, \ldots, K$$

$$Q_k(f^K, f^K) = \sum_{i,j=0}^{K} S_{ijk} Q(\hat{f}_i, \hat{f}_j),$$

$$\text{where } S_{ijk} = \int_{I_{\mathbf{z}}} b(\mathbf{z}) \Phi_i(\mathbf{z}) \Phi_j(\mathbf{z}) \Phi_k(\mathbf{z}) \pi(\mathbf{z}) \mathrm{d}\mathbf{z}.$$

Curse of dimension

- Boltzmann is already 6 dimension in space and velocity; random inputs add many more dimensions
- SG basis for random space:

  if polynomial of degree n is used, then the number of basis is $\binom{n+d}{d}$

Sparse Grids[2]

- Efficient methods to choose basis functions $\{\Phi_k(\mathbf{z})\}$ in high dimensional random spaces
- Guo and Cheng[3] use sparse grids for a discontinuous Galerkin method for transport equations
- For sufficiently smooth function, the approximation error is $O(K^{-(m+1)}(\log K)^{(m+2)(d-1)+1})$ where K is the number of basis, and m is the degree of polynomials.
- Partly break "the curse of dimensionality"

[2] H.-J. Bungartz and M. Griebel, 2004
[3] W. Guo and Y. Cheng, 2016

- Restrict to the case $I_{\mathbf{z}} = [-1,1]^d$, and $\pi(\mathbf{z}) = \frac{1}{2^d}$
- $P^m(a,b)$: the space of polynomials of degree at most m on the interval (a,b)
- Start with 1-d piecewise polynomial space

$$V_N^m = \{\phi : \phi \in P^m(-1+2^{-N+1}j, -1+2^{-N+1}(j+1)), j = 0,1,\ldots,2^N-1\}.$$

- Define W_N^m as the orthogonal complement of V_{N-1}^m inside V_N^m. Then $V_N^m = \oplus_{0\le j\le N} W_j^m$
- Dimension of W_N^m is $(m+1)2^{N-1}$

- In d-dimensional random space, define tensor grids $\mathbf{V}_{N,\mathbf{z}}^m = V_{N,z_1}^m \times \cdots \times V_{N,z_d}^m$. $\mathbf{W}_{\mathbf{j},\mathbf{z}}^m = W_{j_1,z_1}^m \times \cdots \times W_{j_d,z_d}^m$

- Then $\mathbf{V}_{N,\mathbf{z}}^m = \oplus_{0 \le |\mathbf{j}|_\infty \le N} \mathbf{W}_{\mathbf{j},\mathbf{z}}^m$.

When all the components of $\mathbf{j}$ are large, the coefficients are very small. But such spaces have a lot of basis functions!

z_2 \ z_1	W_0^0	W_1^0	W_2^0	W_3^0	W_4^0
W_0^0	1	1	2	4	8
W_1^0	1	1	2	4	8
W_2^0	2	2	4	8	16
W_3^0	4	4	8	16	32
W_4^0	8	8	16	32	64

- Idea: take $\hat{\mathbf{V}}_{N,\mathbf{z}}^m = \oplus_{0 \le |\mathbf{j}|_1 \le N} \mathbf{W}_{\mathbf{j},\mathbf{z}}^m$.
- The most expensive parts are dropped, without affecting the accuracy too much
- 256 → 48 !
- More effective in higher dimensional random spaces

$z_2 \backslash z_1$	$\mathbf{W}_0^0$	$\mathbf{W}_1^0$	$\mathbf{W}_2^0$	$\mathbf{W}_3^0$	$\mathbf{W}_4^0$
$\mathbf{W}_0^0$	1	1	2	4	8
$\mathbf{W}_1^0$	1	1	2	4	8
$\mathbf{W}_2^0$	2	2	4	8	16
$\mathbf{W}_3^0$	4	4	8	16	32
$\mathbf{W}_4^0$	8	8	16	32	64

Number of Basis Functions Sparse vs. Full

(a) $m = 0$

	$N = 3$	$N = 4$	$N = 5$
$d = 1$	8,8	16,16	32,32
$d = 2$	20,64	48,256	112,1024
$d = 3$	38,512	104,4096	272,32768
$d = 4$	63,4096	192,65536	552,1048576

(b) $m = 1$

	$N = 3$	$N = 4$	$N = 5$
$d = 1$	16,16	32,32	64,64
$d = 2$	80,256	192,1024	448,4096
$d = 3$	304,4096	832,32768	2176,262144

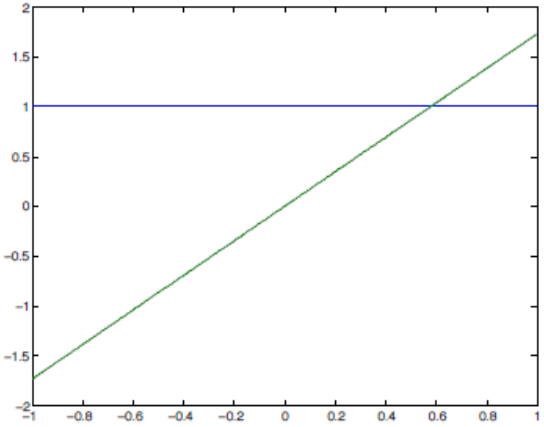
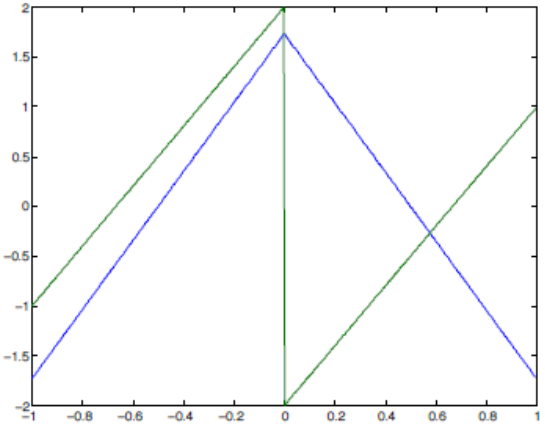
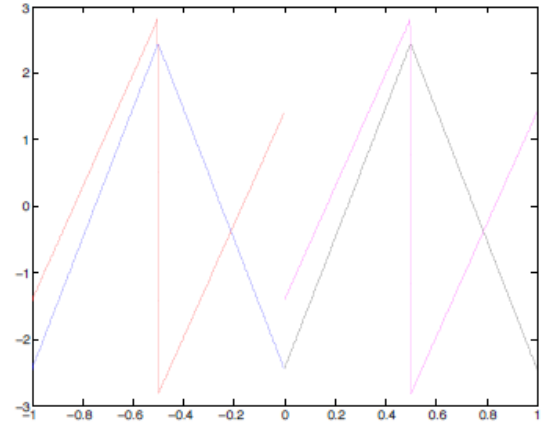
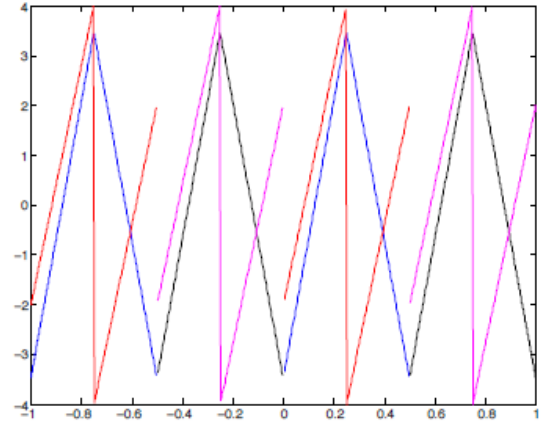
Table 1: Comparison of basis function: d is the dimension; in each cell, the left number (blue) is the number of basis of functions of $\hat{\mathbf{V}}_N^m$; the right number (red) is the number of basis of functions of $\mathbf{V}_N^m$

Sparse grid: $O((m+1)^d 2^N N^{d-1})$

Full grid: $O((m+1)^d 2^{Nd})$

Construct Basis Functions[4]

- Basis functions of W_N^m are locally supported piecewise polynomials
- Basis functions of $\mathbf{W}_N^m$ are tensor products of basis of W_N^m

[4] B. Alpert, 1993

go to 19

Sparsity of S_{ijk}

- The most expensive part is the computation of

$$Q_k(f^K, f^K) = \sum_{i,j=0}^{K} S_{ijk} Q(\hat{f}_i, \hat{f}_j), \quad k = 0, 1, \ldots, K$$

$$\text{where } S_{ijk} = \int_{I_{\mathbf{z}}} b(\mathbf{z}) \Phi_i(\mathbf{z}) \Phi_j(\mathbf{z}) \Phi_k(\mathbf{z}) \pi(\mathbf{z}) \mathrm{d}\mathbf{z}.$$

- The computation of $Q(\hat{f}_i, \hat{f}_j)$ is unnecessary if

$$S_{ijk} = 0, \quad \forall k$$

- This happens if Φ_i and Φ_j have disjoint supports

- Since Φ_i and Φ_j are tensor products of locally supported functions, their supports are disjoint if one of their components are disjoint.

Theorem. *The pairs of basis functions of* $\hat{\mathbf{V}}_N^m$ *with intersecting support have total number at most* $O((m+1)^{2d}2^{2N}N^{d+1})$.
(among $O((m+1)^{2d}2^{2N}N^{2d-2})$ *pairs)*

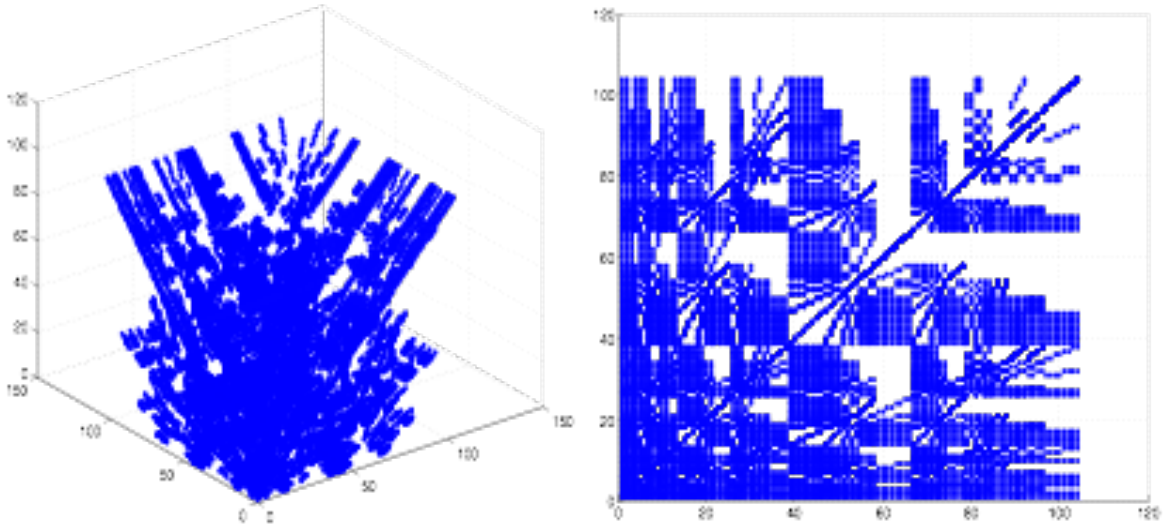


Figure 3: Demonstration of sparsity of S_{ijk}: $m = 0, N = 4, d = 3$

Regularity in the random space

- **Theorem.** *Assume that B depends on $\mathbf{z}$ linearly, B and $\partial_{\mathbf{z}} B$ are locally integrable and bounded in $\mathbf{z}$. Assume $\sup_{\mathbf{z}\in I_{\mathbf{z}}} \|f^0\|_{L^1_{\mathbf{v}}} \le M$, $|||f^0|||_k < \infty$ for some integer $k \ge 0$. Then there exists a constant $C_k > 0$, depending only on B, M, T, and $|||f^0|||_k$ such that*

$$|||f|||_k \le C_k, \qquad \text{for any} \quad t \in [0,T]\,.$$

- $$|||f(t,\cdot,\cdot)|||_k = \sup_{\mathbf{z}\in I_{\mathbf{z}}} \left(\sum_{|\mathbf{l}|=0}^{k} \|\partial_{\mathbf{z}}^{\mathbf{l}} f(t,\mathbf{v},\mathbf{z})\|^2_{L^2_{\mathbf{v}}} \right)^{1/2}$$

Projection Error

- Number of basis functions of $\hat{\mathbf{V}}_N^m$ is $K = O((m+1)^d 2^N N^{d-1})$.
- **Lemma.**[3] *For any* $f \in \mathcal{H}^{m+1}(I_{\mathbf{z}})$, $N \geq 1$, *we have*

$$\|P_K f - f\|_{L^2(I_{\mathbf{z}})} \leq (C(m)N)^d 2^{-N(m+1)} \|f\|_{\mathcal{H}^{m+1}(I_{\mathbf{z}})}.$$

- Express the error in terms of K ,

$$\|P_K f - f\|_{L^2(I_{\mathbf{z}})} \leq C(m,d) K^{-(m+1)} (\log K)^{(m+2)(d-1)+1} \|f\|_{\mathcal{H}^{m+1}(I_{\mathbf{z}})}.$$

- The space $\mathcal{H}^m(I_{\mathbf{z}})$ is defined by $\|f\|_{\mathcal{H}^m(I_{\mathbf{z}})} = \max \|\partial_{z_{i_1}}^m \cdots \partial_{z_{i_r}}^m\|_{L^2(I_{\mathbf{z}})}$

[3] W. Guo, Y. Cheng, 2016

Accuracy estimate

Theorem. *Assume the random variable z and initial data f^0 satisfy the assumption in the lemma for regularity, and the Galerkin approximation f^K is uniformly bounded in K, then*

$$\|f-f^K\|_{L^2_{v,z}} \leq C(t)\left\{C(m,d)K^{-(m+1)}(\log K)^{(m+2)(d-1)+1}+\|e^K(0)\|_{L^2_{v,z}}\right\},$$

where $e^K(0)=(P_Kf-f^K)|_{t=0}$.

Numerical Result 1: Approximation Error

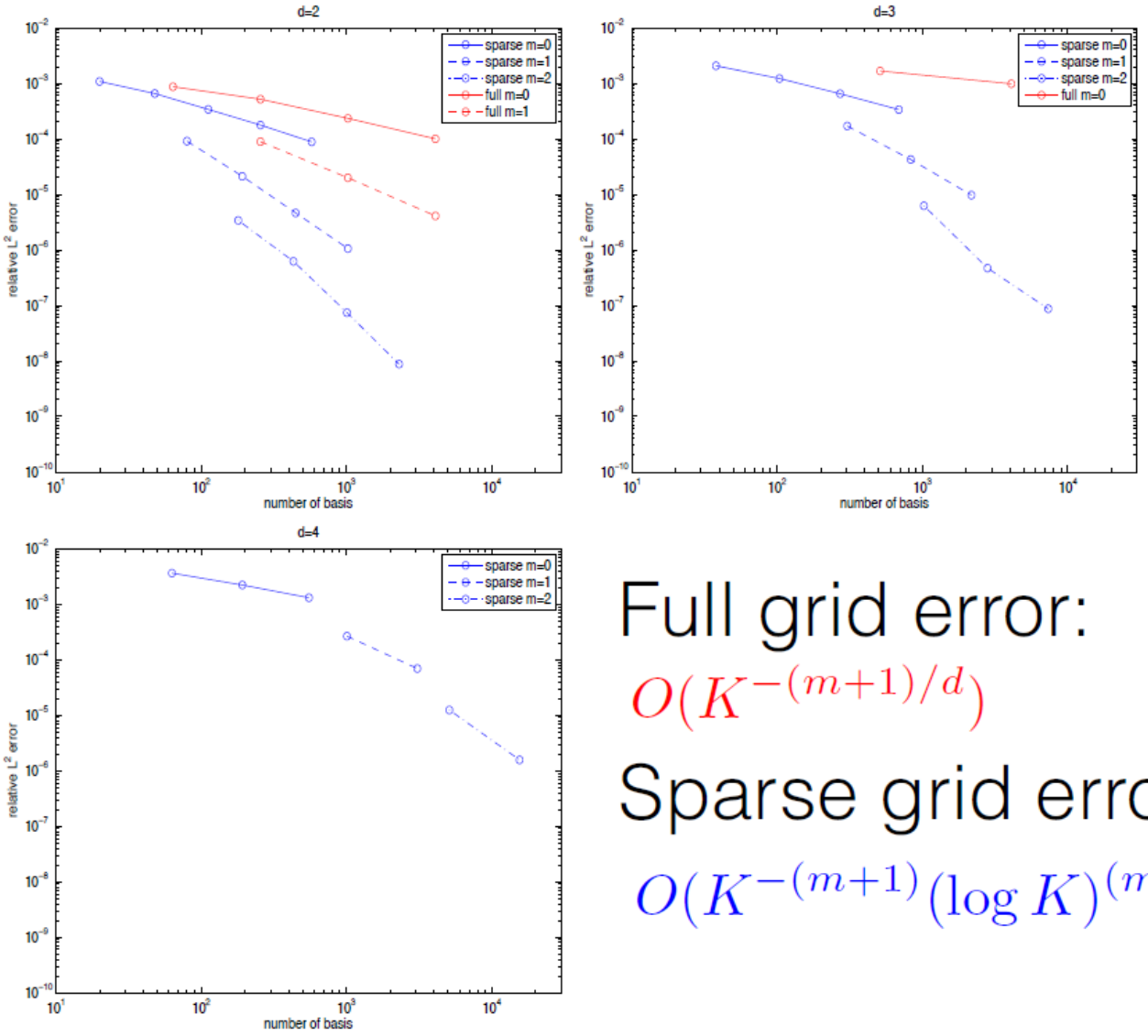
- Take function $f(\mathbf{z})$ in random spaces with dimension 2, 3, 4

$$f(\mathbf{z}) = \frac{1}{2\pi\mathcal{K}(\mathbf{z})^2}\exp\left(-\frac{1}{2\mathcal{K}(\mathbf{z})}\right)\left(2\mathcal{K}(\mathbf{z}) - 1 + \frac{1-\mathcal{K}(\mathbf{z})}{2\mathcal{K}(\mathbf{z})}\right),$$

where

$$\mathcal{K}_{d=2}(\mathbf{z}) = 1 - 0.5(0.5 + 0.1\sin(z_1) + 0.1\sin(2z_2)),$$
$$\mathcal{K}_{d=3}(\mathbf{z}) = 1 - 0.5(0.5 + 0.1\sin(z_1) + 0.1\sin(2z_2) + 0.1\cos(z_3)),$$
$$\mathcal{K}_{d=4}(\mathbf{z}) = 1 - 0.5(0.5 + 0.1\sin(z_1) + 0.1\sin(2z_2) + 0.1\cos(z_3) + 0.1\cos(2z_4)).$$

- Compare relative error $\frac{\|f - Pf\|_{L^2}}{\|f\|_{L^2}}$



Full grid error:

$$O(K^{-(m+1)/d})$$

Sparse grid error:

$$O(K^{-(m+1)}(\log K)^{(m+2)(d-1)})$$

Figure 1: Comparison of approximation error for $d = 2, 3, 4$. For $d = 4$ we do not give the result by tensor grid because the number of basis functions is too large.

Numerical Result 2: Solve BE with uncertainty

- **6**-dimensional random space. 3 for initial data, 2 for boundary data, 1 for collision kernel. 1-d in $\mathbf{x}$, 2-d in $\mathbf{v}$
- Initial data: equilibrium with

$$\rho(x,\mathbf{z})=1,\quad \mathbf{u}(x,\mathbf{z})=0,\quad T=1+0.5(1+0.2z_2)\exp(-100(1+0.1z_3)(x-0.4-0.01z_1)^2)$$

- Boundary data: at $x=0$ take Maxwell boundary with

$$T_w=1+0.2z_4,\quad \alpha=0.5+0.3z_5.$$

- Collision kernel: $b(\mathbf{z})=1+0.2z_6$
- Take sparse grid basis with $m=0, N=3$, number of basis: 138
- Compare with stochastic collocation method at $t=0.04$

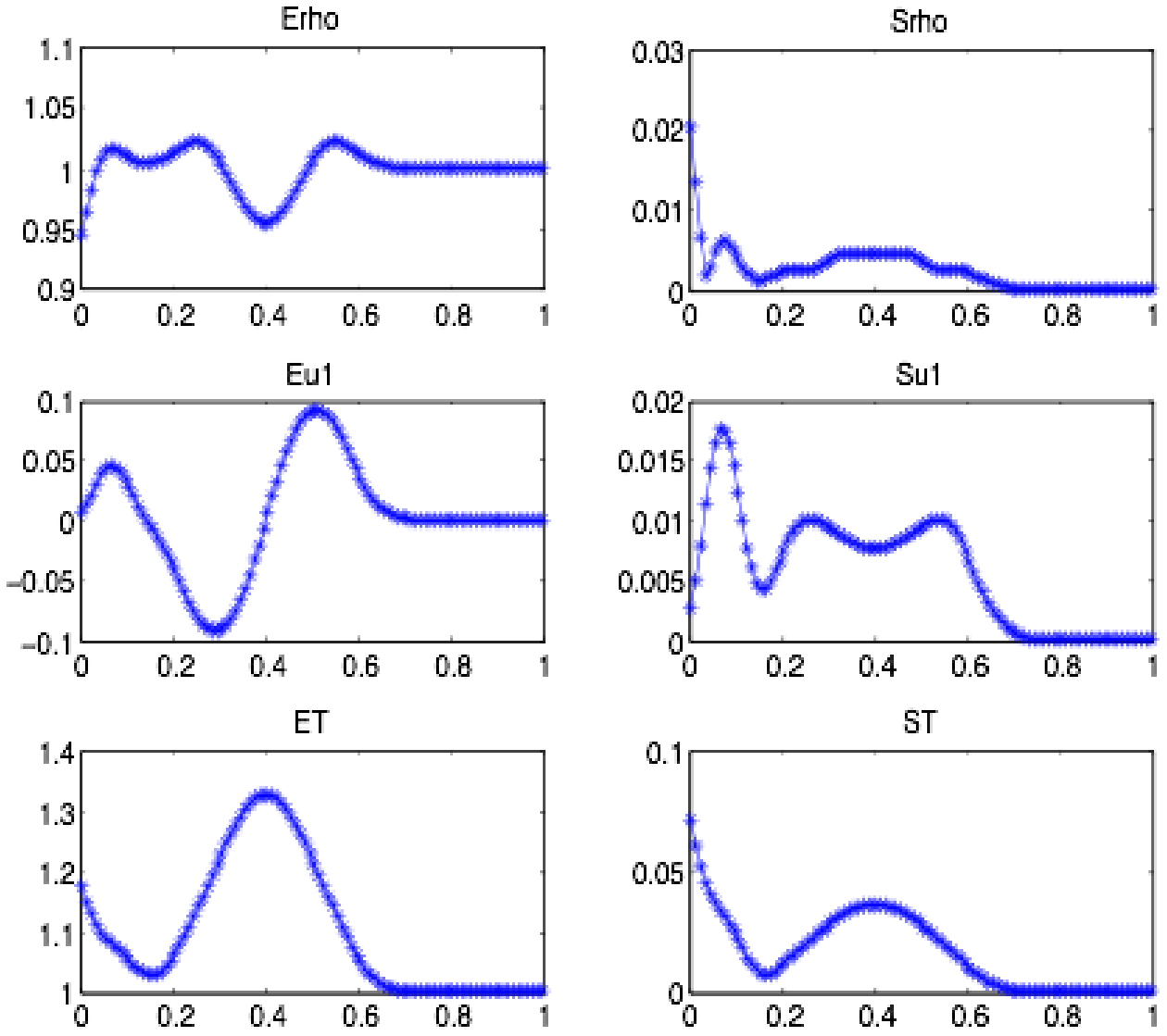


Figure 7: Inhomogeneous Boltzmann equation with randomness on initial data, boundary data, and collision kernel ($d = 6$). Curve: collocation; asterisks: Galerkin.

gPC-SG for many different kinetic equations

- Boltzmann: a fast algorithm for collision operator (J. Hu-Jin, JCP '16), sparse grid for high dimensional random space (J. Hu-Jin-R. Shu '16): initial regularity in the random space is preserved in time; but not clear whether it is 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, '16): not able to prove regularity result in the random space (APUQ is open)
- Semiconductor Boltzmann-drift diffusion limit (uniform regularity. APUQ OK: Jin-L. Liu '15)
- Radiative heat transfer (APUQ OK: Jin-H. Lu '16): proof of regularity in random space for linearized problem (nonlinear? Open)
- Valsov-Poisson-Fokker-Planck equation and high field limit (APUQ OK in 1D: Jin-Y. Zhu '16): proof of regularity in random space for linearized problem (nonlinear? Open)

conclusion

- gPC-SG allows us to treat kinetic equations with random inputs in the deterministic AP framework
- Many different kinetic equations can be solved this way;
- Rigorous sharp s-AP analysis established for linear transport equation.
- Kinetic equations have the good regularity in the random space, even for the nonlinear Boltzmann equation (Hu-Jin '16)
- Many kinetic ideas useful for UQ problems: mean-field approximations; moment closure; etc. （APUQ is one example）
- Some of the estimates/techniques for velocity space can be used in random space
- Many open questions, very few existing works
- Kinetic equations are good problems for UQ;

** UQ + Multiscale **