# Uncertainty Quantification for multiscale kinetic equations with random inputs IV

Shi Jin

University of Wisconsin-Madison, USA
Shanghai Jiao Tong University, China

# VI. High dimensional random space (R. Shu-J. Hu-J, Num. Math '17)

## 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"

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

- Restrict to the case $I_{\mathbf{z}} = [-1,1]^d, \text{ and } \pi(\mathbf{z}) = \frac{1}{2^d}$

- $P^m(a,b)$ : 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 $\mathbf{V}^m_{N,\mathbf{z}} = V^m_{N,z_1} \times \cdots \times V^m_{N,z_d}$. $\mathbf{W}^m_{\mathbf{j},\mathbf{z}} = W^m_{j_1,z_1} \times \cdots \times W^m_{j_d,z_d}$
- Then $\mathbf{V}^m_{N,\mathbf{z}} = \oplus_{0\le|\mathbf{j}|_\infty\le N} \mathbf{W}^m_{\mathbf{j},\mathbf{z}}$.

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

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

- Idea: take $\hat{\mathbf{V}}^m_{N,\mathbf{z}} = \oplus_{0\leq|\mathbf{j}|_1\leq N}\mathbf{W}^m_{\mathbf{j},\mathbf{z}}$.

- The most expensive parts are dropped, without affecting the accuracy too much

- 256 → 48 !

- More effective in higher dimensional random spaces

| $z_2 \backslash z_1$ | $\mathbf{W}^0_0$ | $\mathbf{W}^0_1$ | $\mathbf{W}^0_2$ | $\mathbf{W}^0_3$ | $\mathbf{W}^0_4$ |
|---|---|---|---|---|---|
| $\mathbf{W}^0_0$ | 1 | 1 | 2 | 4 | 8 |
| $\mathbf{W}^0_1$ | 1 | 1 | 2 | 4 | 8 |
| $\mathbf{W}^0_2$ | 2 | 2 | 4 | 8 | 16 |
| $\mathbf{W}^0_3$ | 4 | 4 | 8 | 16 | 32 |
| $\mathbf{W}^0_4$ | 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: $O((m+1)^d 2^{Nd})$

# Sparsity of $S_{ijk}$

- The most expensive part is the computation of

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

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 $\Phi_i$ and $\Phi_j$ have disjoint supports

- Since $\Phi_i$ and $\Phi_j$ are tensor products of locally supported functions, their supports are disjoint if one of their components are disjoint.

**Theorem 4.1.** *The pairs of basis functions of $\hat{\mathbf{V}}_N^m$ with intersecting supports have a total number at most $O((m+1)^{2d}2^{2N}N^{d+1})$.*

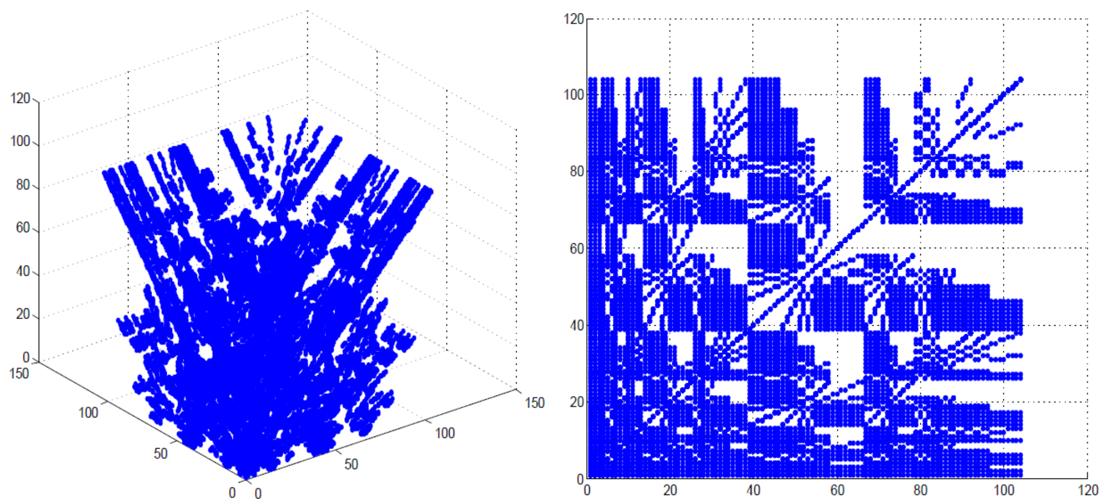



Figure 3: Demonstration of sparsity of $S_{ijk}$: $m = 0, N = 4, d = 3$.

# 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* $\sup_{\mathbf{z}\in I_{\mathbf{z}}} \|f^0\|_{L^1_{\mathbf{v}}} \leq M$, $\||f^0\||_k < \infty$ *for some integer* $k \geq 0$*. Then there exists a constant* $C_k > 0$*, depending only on* $B$*,* $M$*,* $T$*, and* $\||f^0\||_k$ *such that*

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

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

# 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* $e^K(0) = (P_K f - f^K)|_{t=0}$.

# Numerical Result 1: Approximation Error

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

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

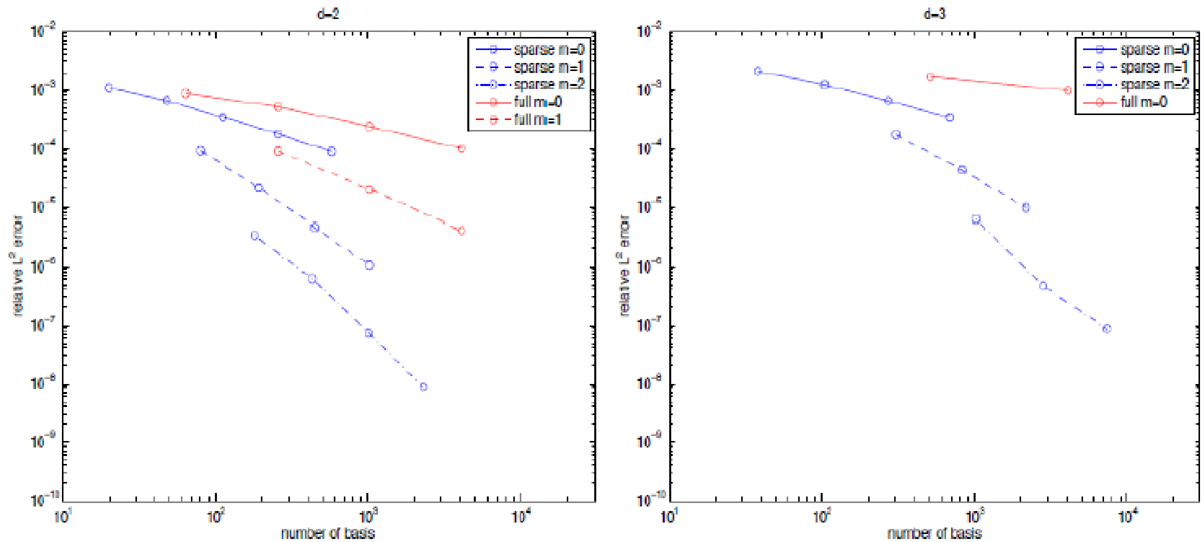
where

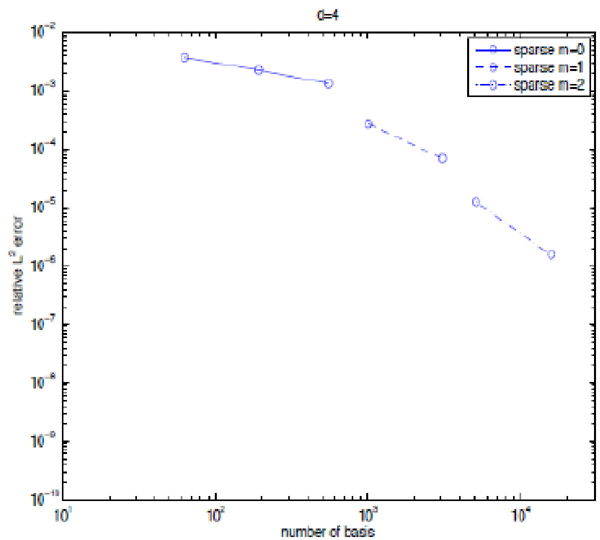
$$\mathcal{K}_{d=2}(\mathbf{z}) = 1 - 0.5(0.5 + 0.1\sin(z_1) + 0.1\sin(2z_2)),$$

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

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

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




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 $t = 0.04$

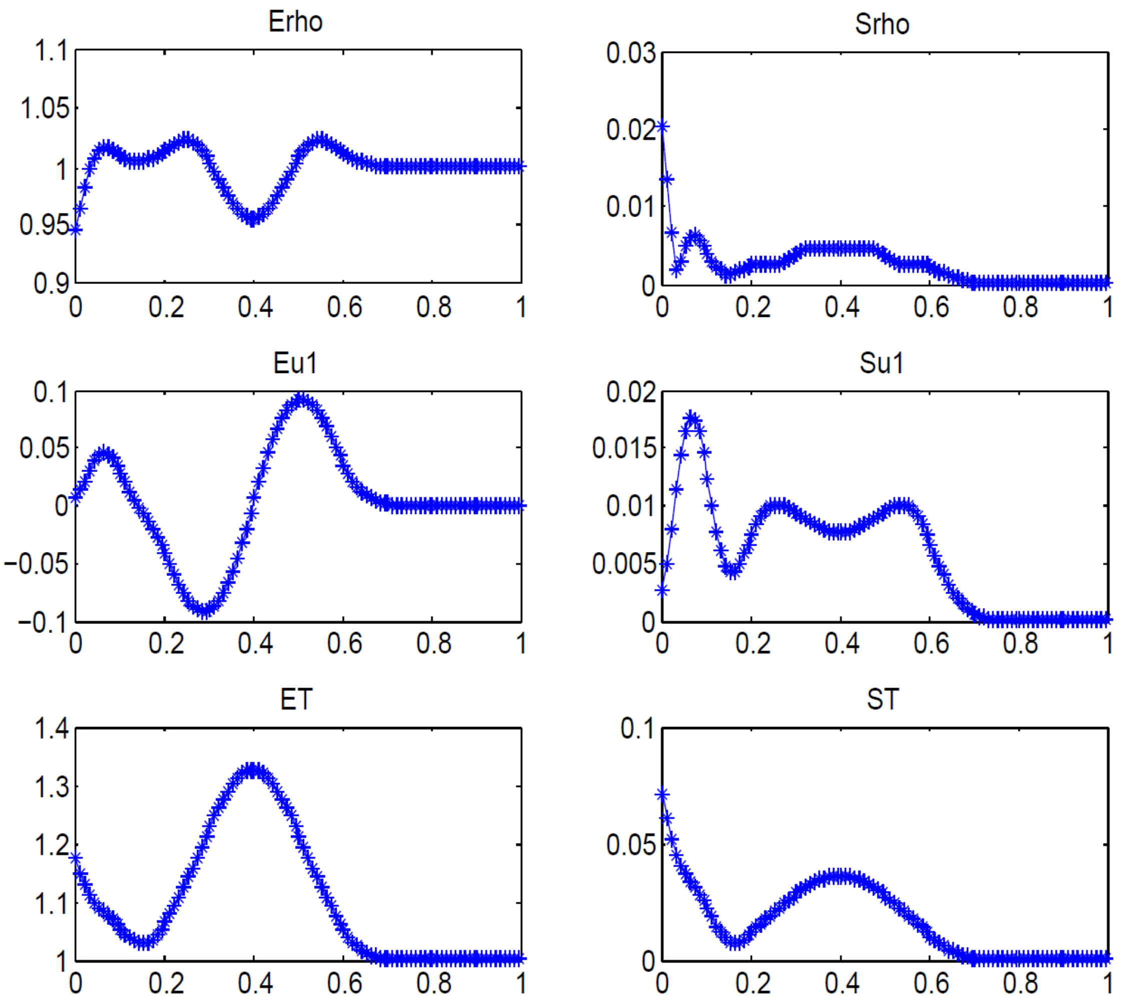



Figure 7: The Boltzmann equation with randomness on initial data, boundary data, and collision kernel ($d = 6$). $N_x = 100$, $t = 0.04$. Curve: collocation with $M_z = 4$; asterisks: Galerkin with $m = 0, N = 3$. Left column: mean of density, first component of bulk velocity, and temperature. Right column: standard deviation of density, first component of bulk velocity, and temperature.

# High dimensional random space (J-Zuazua-Y. Zhu)

- Consider random parametric linear Vlasov-Fokker-Planck equation

$$\epsilon\partial_t f + v\partial_x f - \partial_x\phi\partial_v f = \frac{1}{\epsilon}\mathcal{F}f, \quad x, v \in \Omega = (0, l) \times \mathbb{R}$$

$$\mathcal{F}f = \partial_v\left(M\partial_v\left(\frac{f}{M}\right)\right) \qquad M(v) = \frac{1}{\sqrt{2\pi}}e^{-\frac{|v|^2}{2}}$$

$$E(x, \mathbf{z}) = \partial_x\phi(x, \mathbf{z}) = \bar{E}(x) + \sum_{j\geq 1} z_j E_j(x),$$

$$\mathbf{z} \in U = [-1, 1]^\infty$$

# Best N-approximation

We seek approximate solution $h_\Lambda$ in a finite dimensional space,

$$\mathbb{P}_\Lambda = \{h_\Lambda : h_\Lambda = \sum_{\nu\in\Lambda} h_\nu(t,x,v)L_\nu(\mathbf{z})\}, \tag{3.1}$$

where $\Lambda$ is an index set with infinite dimensional vectors $\nu$. Here $L_\nu(\mathbf{z})$ form the normalized Legendre polynomial basis such that,

$$L_\nu = \prod_{j\geq 1} L_{\nu_j}(z_j), \quad \int_{-1}^{1} L_k(z_j)L_l(z_j)\frac{dz_j}{2} = \delta_{kl}, \tag{3.2}$$

so $L_\nu$ is also an orthogonal basis in $L^2(U,d\rho)$.

the projection of the solution $h$ onto $\mathbb{P}_\Lambda$,

$$P_\Lambda h = \sum_{\nu\in\Lambda}\left(\int_U hL_\nu d\rho\right)L_\nu := \sum_{\nu\in\Lambda} h_\nu L_\nu = \operatorname*{argmin}_{h_\Lambda\in\mathbb{P}_\Lambda} \|h-h_\Lambda\|_{L^2(U,V,d\rho)}.$$

The best N approximation is a form of nonlinear approximation that searches for $\nu\in\Lambda$ according to the largest $N$ coefficients $\|h_\nu\|_V$

# Cohen-Devore-Schwab ('10)

**Theorem 3.1** (Corollary 3.11 of [3]). *Consider a parametric problem of the form*

$$\mathcal{P}(f, a) = 0, \tag{3.4}$$

*with random field* $a = \bar{a}(x) + \sum_{j \geq 1} z_j \psi_j(x) \in X$, $\mathbf{z} \in U$, *where* $X$ *is certain space of* $x$. *Assume the solution map* $a \to f(a)$ *admits a holomorphic extension to an open set* $\mathcal{O} \in X$ *which contains* $a(U) = \{a(\mathbf{z}) : \mathbf{z} \in U\}$, *with uniform bound*

$$\sup_{a \in \mathcal{O}} \|u(a)\|_V \leq C. \tag{3.5}$$

*If in addition* $\left(\|\psi_j\|_X\right)_{j \geq 1} \in \ell^p(\mathbb{N})$ *for some* $p < 1$, *then for the set of indices* $\Lambda_n$ *that corresponds to the* $n$ *largest* $f_\nu = \left\|\int f L_\nu d\rho\right\|_V$, *one has,*

$$\left\| f - \sum_{\nu \in \Lambda_n} f_\nu L_\nu \right\|_{L^2(U,V,\rho)} \leq \frac{C}{(n+1)^s}, \quad s = \frac{1}{p} - \frac{1}{2} \tag{3.6}$$

*where* $C := \| \|f_\nu\|_V \|_{\ell^p}$.

- While C-D-S proved it for elliptic PDEs, we extend it to linear Vlasov-Fokker-Planck equations with random forcing
- 1) assume isotropy

**Condition 2.1.** *Assume* $\|\partial_x E\|_{L^\infty(U,L^\infty_x)}, \|E\|_{L^\infty(U,L^\infty_x)} \leq C_E$; $\|\partial_x E_j\|_{L^\infty_x}, \|E_j\|_{L^\infty_x} \leq C_j$. *Furthermore, the upper bounds* $C_E, C_j$ *satisfies,*

$$C_E + \sum_{j\geq 1} C_j \leq \min\left\{\frac{2\lambda}{7}, \frac{C_s}{2}\right\}, \quad C_E \leq \frac{\lambda C_s}{48}, \tag{2.16}$$

$$\sum_{j\geq 1} \sqrt{C_j} \leq \sqrt{\frac{\lambda C_s}{8}}, \quad (C_j)_{j\geq 1} \in l^{\frac{p}{2}}(\mathbb{N}), \text{ for some } p \leq 1. \tag{2.17}$$

- 2) prove analyticity

**Theorem 3.2.** *Under Condition 2.1, for* $\forall \mathbf{z} \in U$, *one has the following estimate for the solution to (2.8),*

$$\|\partial^\nu h(t)\|_V \leq B(t)\,(|\nu|!)\,b^\nu. \tag{3.8}$$

*where* $b$ *is an infinite dimensional vector with the* $j$*-th component*

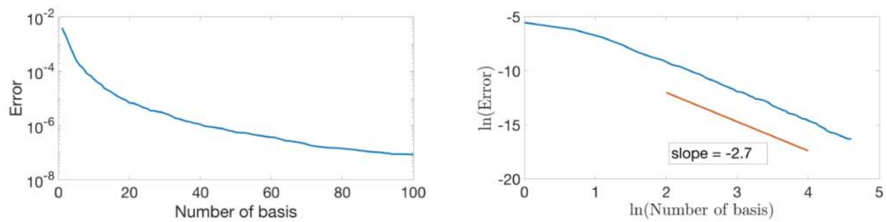
$$b_j = \sqrt{\frac{3C_j}{2C_3}}, \tag{3.9}$$

$B(t)$ *is an exponential decay function in* $t$,

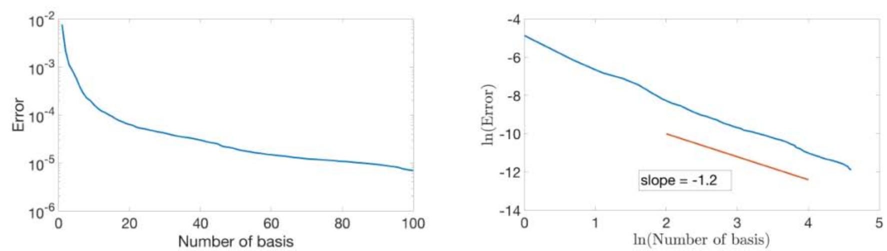
$$B(t) = \min\left\{\frac{2}{\epsilon}\|h(0)\|_V\, e^{-\frac{2C_3}{\epsilon^2}t}, 2\,\|h(0)\|_V\, e^{-2C_3 t}\right\}, \tag{3.10}$$

$C_3 = \frac{\lambda C_s}{16}$, $C_s, \lambda$ *are constants defined in (1.1), (2.10).*

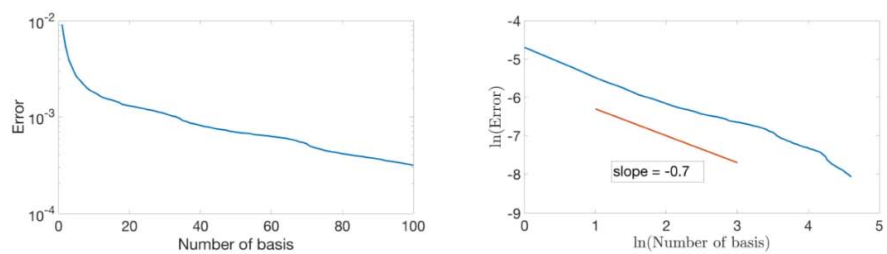
# Numerical tests




(a) The convergence rate for the case of $E(x,\mathbf{z}) = \frac{\sin(x)}{2} + \sum_{j=1}^{100} \frac{\cos(jx)}{2^j} z_j$




(b) The convergence rate for the case of $E(x,\mathbf{z}) = \frac{\sin(x)}{2} + \sum_{j=1}^{100} \frac{\cos(jx)}{j^2} z_j$




(c) The convergence rate for the case of $E(x,\mathbf{z}) = \frac{\sin(x)}{2} + \sum_{j=1}^{100} \frac{\cos(jx)}{j} z_j$

**Figure 1:** This is the convergence rate of the approximate solution to (4.29) at $t = 1$ with different parametric forcing terms obtained by Algorithm 4.1, where we set $\epsilon = 1$.

# Kinetic equations vs Uncertainty Quantification

| Kinetic equations | Uncertainty Quantification |
| --- | --- |
| • PDEs in phase space with velocity | • PDEs with parameters |
| • Polynomial chaos based stochastic Galerkin (loss of hyperbolicity for nonlinear hyperbolic systems) | • Grad's thirteen moment closure (via Hermite polynomials) (loss of hyperbolicity) |
| • Dimension reduction: mean-field limit, molecular chaos-BBGKY etc. | • Dimension reduction: low rank perturbation; evolution of marginal distribution, … |
| • Particles to kinetic equations | • Stochastic gradient decent to Fokker-Planck equation |
| • AP | • sAP |

# Open questions

- For SG for Boltzmann, in the fluid limit, one arrives at a SG for compressible Euler. Hyperbolicity? ( a direct application of SG for Euler loses hyperbolicity)
- Sharper estimate? Remove linearity assumption in z, stronger perturbation, more general random variables and orthogonal polynomials
- Landau damping under uncertainty (preliminary results by R. Shu-J on regularity of solution in random space)
- Control and inverse problems (regularization based or Bayesian inference theory based)
- Utilize sparsity to reduce computational costs
- Machine learning techniques
- Other applications