A bi-fidelity method for kinetic models with uncertainties

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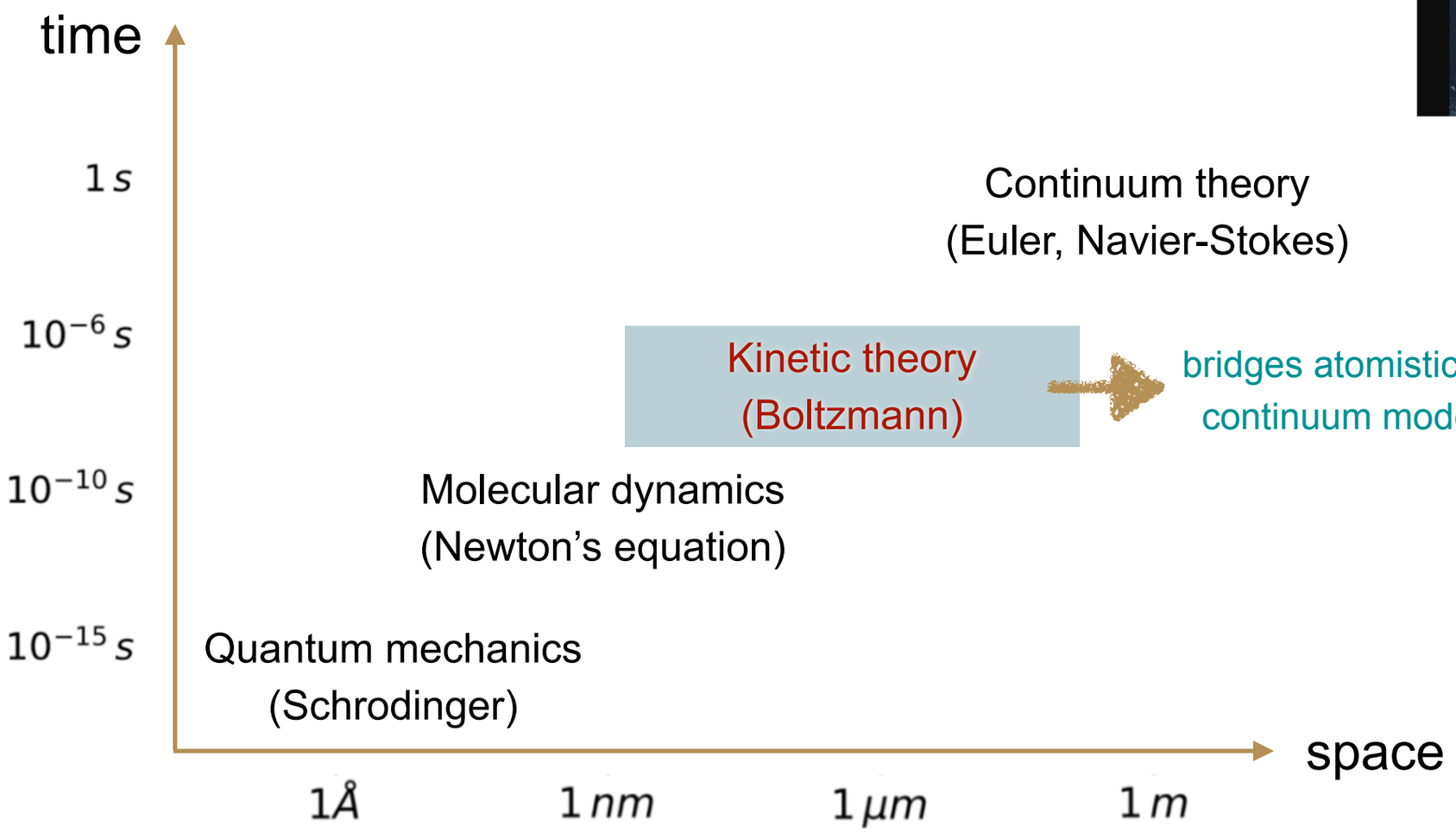
Outline

- Background on Uncertainty Quantification (UQ) for kinetic equations
- A bi-fidelity stochastic collocation method
- Numerical examples for the Boltzmann and linear transport model
- Error and convergence analysis
- Conclusion

Kinetic equations



A hierarchy of multiscale modeling

Applications:

- Rarefied gas: Boltzmann equation
- Plasma (Vlasov-Poisson, Landau, Fokker-Planck)
- Semiconductor device modeling
- Nuclear reactor (neutron transport), radiative transfer
- Biology
- Collective behavior in biological and social sciences, etc.

UQ for kinetic equations

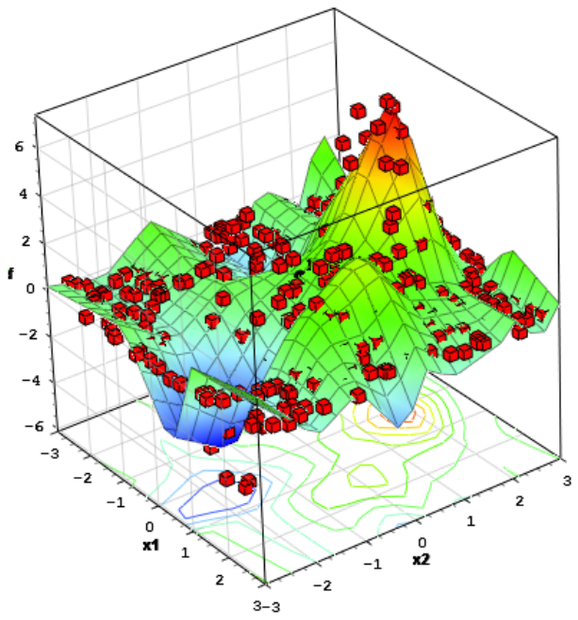
* **UQ:** Quantifying the uncertainties is important to *assess, validate and improve* the underlying models.
* Most modeling of physical systems contain various sources of uncertainties.
* Kinetic equations: usually derived from N-body Newton's second law, mean-field limit etc, the modeling itself is *uncertain.*

* **Parametric uncertainty:**

Collision kernels are often *empirical*, due to incomplete knowledge of the interaction mechanism; inaccurate measurement of the initial and boundary data, etc.

* Despite its popularity in solid mechanics, elliptic equations (Abgrall, Babuska, Ghanem, Gunzburger, Hesthaven, Karniadakis, Mishra, Xiu, Webster, Schwab etc), *few efforts on UQ for kinetic equations have been done until recent years.*

Stochastic Collocation



$$\{z_j, u(z_j)\}_{j=1}^{N_p} \rightarrow u_N(Z) = u(Z)$$

expensive to obtain for large N

Interpolation/quadrature rule based on gPC expansion,

- ☑ Non-intrusive
- ☑ Fast convergence for smooth problems

However,

- The deterministic code is too computationally expensive
- Curse of dimensionality when d >>1

In general, this class of problem is **challenging.** There are attempts in:

- Sparse grid, sparse wavelet basis, compressed sensing, ….

High cost: repetitive runs of deterministic solvers

Problem setup

$$\begin{cases} u_t(x,t,Z) = \mathcal{L}(u), & \text{in } D \times (0,T] \times I_Z, \\ \mathcal{B}(u) = 0, & \text{on } \partial D \times [0,T] \times I_Z, \\ u = u_0, & \text{in } D \times \{t=0\} \times I_Z. \end{cases}$$

u^L : low fidelity solution (cheap)

u^H : high fidelity solution (expensive)

The goal: build a surrogate of u^H in a non-intrusive way

$$v(x,t,z) = \sum_{n=1}^{m} c_n(z) u^H(x,t,z_n), \quad z_n \in I_Z$$

Q1: How to choose z_n intelligently?

Q2: How to compute c_n without extensive sampling from the high-fidelity model?

* A.Narayan, C.Gittelson, D.Xiu 14'

Point selection

Key idea: Explore the parameter space by using the cheap low-fi model

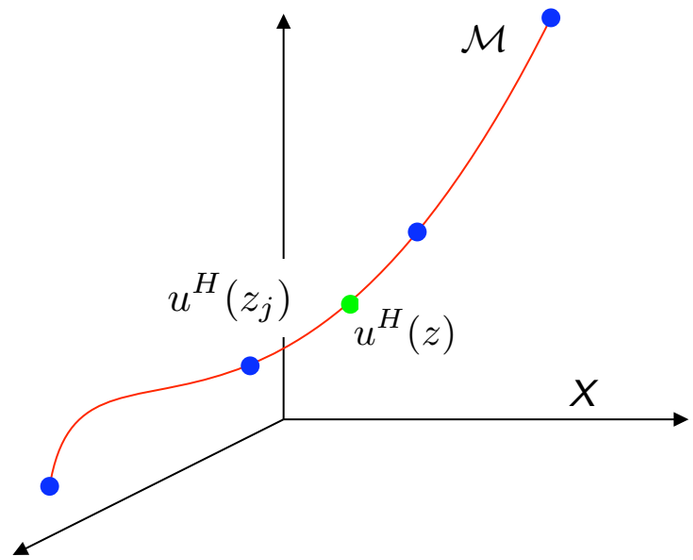
✦ Search the space by the low-fi model via *greedy algorithm:*

$$z_m = \arg\max_{z\in\Gamma} d(u^L(z), U^L_{m-1})$$

Candidate set: $\Gamma = \{z_1, \ldots, z_M\}$

Low-fi approximation space:

$$U^L_{m-1}(\gamma) = \{u^L(z_1), \ldots, u^L(z_{m-1})\}$$



- Enrich the space by finding the *furtherest point* away from the space spanned by the existing set
- The greedy choice is (almost) optimal (DeVore 13').

Lifting procedure

* Construct $\{c_n\}$ as *projection coefficients* from low-fidelity model:

$$v(z)^L = \mathcal{P}_{U^L(\gamma)} u^L(z) = \sum_{n=1}^{m} c_n(z) u^L(z_n)$$

$$\mathbf{G}^L \mathbf{c} = \mathbf{f}, \qquad \mathbf{f} = (f_k)_{1 \le k \le N}, \qquad f_k = \langle u^L(z), u^L(z_{i_k}) \rangle^L,$$

where $\mathbf{G}^L$ is the Gramian matrix of $u^L(\gamma_N)$, defined by

$$(\mathbf{G}^L)_{ij} = \langle u^L(z_{i_k}), u^L(z_{j_k}) \rangle^L, \qquad 1 \le k, i, j \le \bar{m}$$

* Using *the same coefficients*, construct the approximation rule for high-fidelity model

$$v(x,t,z)^H = \sum_{n=1}^{m} c_n(z) u^H(z_n)$$

- This is in fact a lifting operator from low-fi space to high-fi space
- Justification: e.g., scalar scaling, coarse/fine mesh

Overview of Bi-fidelity algorithm

- Run the low-fi models at each point of Γ to obtain $u^L(\Gamma), U^L(\Gamma)$

  select the most "important" m points — γ

Offline

* Run the high-fi models on those m points to get $u^H(\gamma)$

most expensive part

- Bi-fidelity approximation:

  * For any given $z \in I_z$, compute low-fi projection coefficients

$$v(z)^L = \mathcal{P}_{U^L(\gamma)} u^L(z) = \sum_{n=1}^{m} c_n(z) u^L(z_n)$$

Online

  * Apply the same coefficients to $u^H(\gamma)$ to get the bi-fi approximation

$$v(z)^H = \sum_{n=1}^{m} c_n(z) u^H(z_n)$$

* This approximation quality depends on how well the low-fi model approximates the functional variation of high-fi model *in the parameter space.*

The Boltzmann equation

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

* f is the probability density distribution function, modeling the probability of finding a particle at time t, position x, velocity v

* ε is the Knudsen number that characterizes *the degree of rarefiedness* of the gas; ratio of mean free path and the characteristic length scale

$\varepsilon \sim O(1)$ kinetic regime; $\varepsilon \ll O(1)$ hydrodynamic regime

* Q is a *quadratic integral operator* modeling binary interaction between particles

* Ludwig Boltzmann, 1872’

Boltzmann collision operator

* *non-linear* double *integral* collision operator; high-dimensional in physical space

$$\mathcal{Q}(f,f)(\mathbf{v}) = \int_{\mathbb{R}^d}\int_{S^{d-1}} B(\mathbf{v}-\mathbf{v}_*,\sigma)[f(\mathbf{v}')f(\mathbf{v}'_*) - f(\mathbf{v})f(\mathbf{v}_*)]\,\mathrm{d}\sigma\mathrm{d}\mathbf{v}_*$$

$(\mathbf{v},\mathbf{v}_*)$ and $(\mathbf{v}',\mathbf{v}'_*)$ are the velocity pairs before and after collision:

$$\begin{cases} \mathbf{v}' = \dfrac{\mathbf{v}+\mathbf{v}_*}{2} + \dfrac{|\mathbf{v}-\mathbf{v}_*|}{2}\sigma \\ \mathbf{v}'_* = \dfrac{\mathbf{v}+\mathbf{v}_*}{2} - \dfrac{|\mathbf{v}-\mathbf{v}_*|}{2}\sigma \end{cases}$$

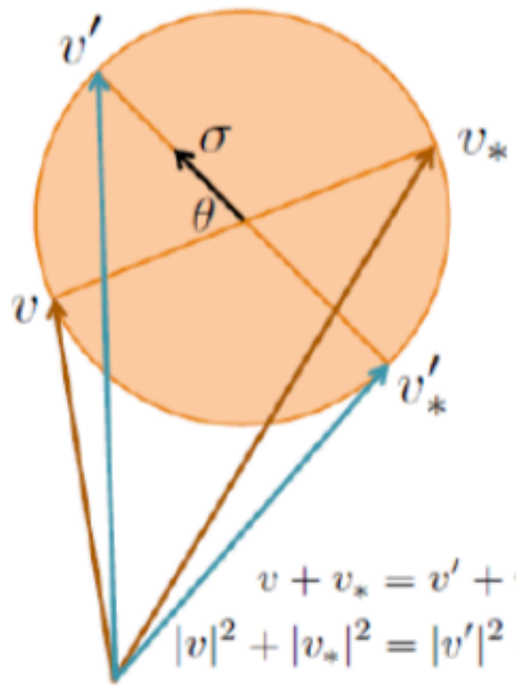
$$B(\mathbf{v}-\mathbf{v}_*,\sigma) = B(|\mathbf{v}-\mathbf{v}_*|, \tfrac{\sigma\cdot(\mathbf{v}-\mathbf{v}_*)}{|\mathbf{v}-\mathbf{v}_*|})$$

Variable hard sphere (VHS) model

$B = b_\lambda|\mathbf{v}-\mathbf{v}_*|^\lambda,\ -d < \lambda \le 1$

$\lambda = 1$: hard sphere molecule

$\lambda = 0$: Maxwell molecule



elastic collisions

Our choice of the low-fidelity model

- Let $\langle \cdot \rangle$ be the velocity averages of the argument,

$$\langle f \rangle = \int_{\mathbb{R}^d} f(v)\, dv.$$

- Multiply the equation

$$\partial_t f + v \cdot \nabla_x f = \frac{1}{\varepsilon} \mathcal{Q}$$

by $m(v) = \left(1, v, \frac{|v|^2}{2}\right)^T$ and integrate on v, then

$$\partial_t \langle mf \rangle + \nabla_x \cdot \langle vmf \rangle = 0.$$

- When $\varepsilon \to 0$, $f \to M(v)_{\rho,u,T}$. Replace f by $M(U)$, the above equation becomes closed and reduces to the compressible Euler equations

$$\partial_t \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} + \nabla_x \cdot \begin{pmatrix} \rho u \\ \rho u \otimes u + p\, I \\ (E+p)u \end{pmatrix} = 0,$$

where E is the total energy defined by

$$E = \langle \frac{1}{2}|v|^2 f \rangle = \frac{1}{2}\rho|u|^2 + \frac{d}{2}\rho T.$$

* Liu-X.Zhu (JCP 19')

Example 1: double peak initial data test

$$
\begin{cases}
\rho_0(x, \mathbf{z}^\rho) = \dfrac{1}{3}\left(2 + \sin(2\pi x) + 0.2\sum_{k=1}^{d_1} \sin[2\pi(k+1)x]\,\dfrac{z_k^\rho}{2k}\right), \\
\mathbf{u}_0 = (0.2, 0), \\
T_0(x, \mathbf{z}^T) = \dfrac{1}{4}\left(3 + \cos(2\pi x) + 0.2\sum_{k=1}^{d_1} \cos[2\pi(k+1)x]\,\dfrac{z_k^T}{2k}\right), \\
f_0(x, \mathbf{v}, \mathbf{z}) = \dfrac{\rho_0}{4\pi T_0}\left(\exp(-\dfrac{|\mathbf{v}-\mathbf{u_0}|^2}{2T_0}) + \exp(-\dfrac{|\mathbf{v}+\mathbf{u_0}|^2}{2T_0})\right).
\end{cases}
\tag{5.3}
$$

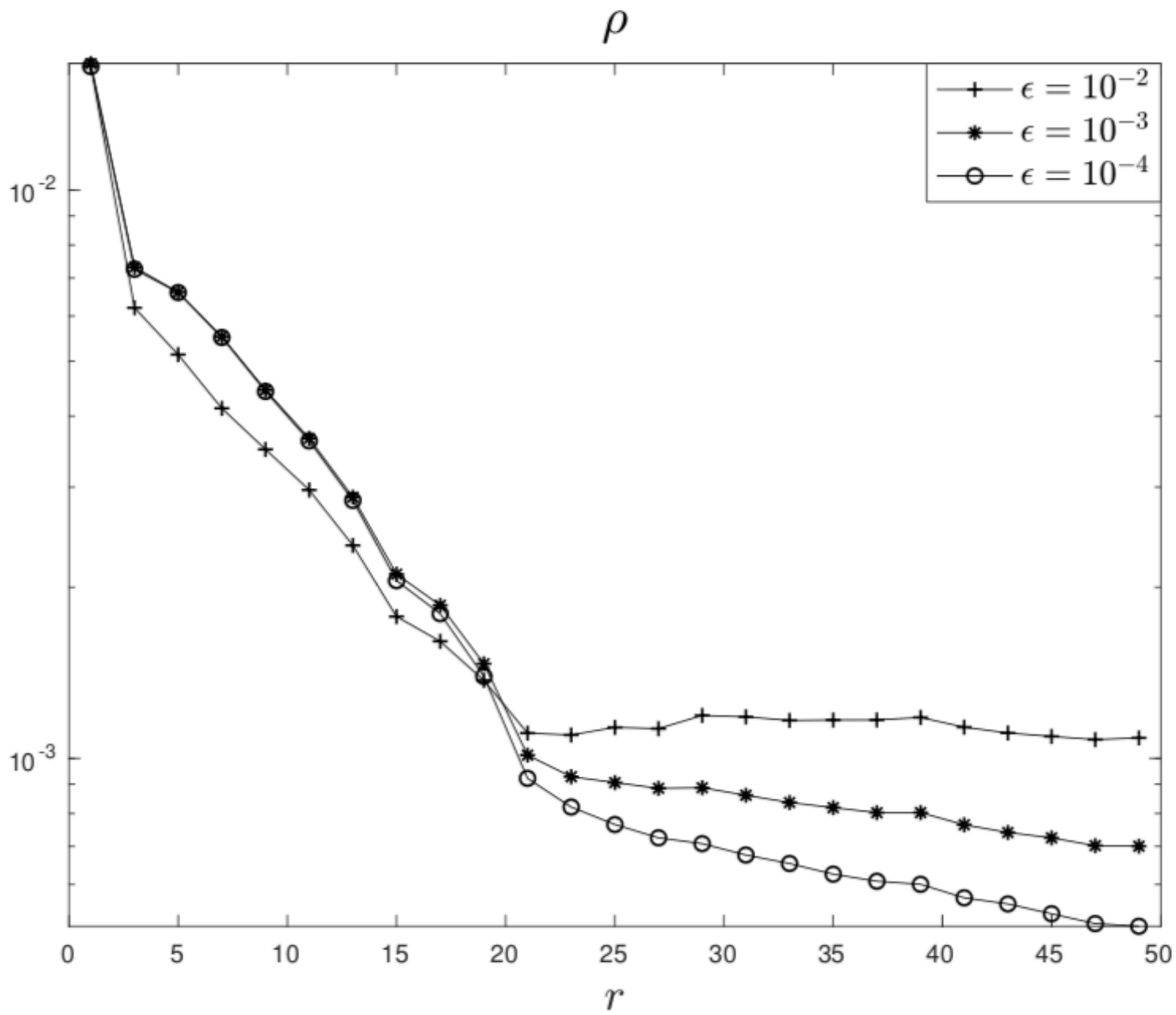
The uncertain collisional cross section is given by

$$
b(z) = 1 + 0.5 z_1^b, \tag{5.4}
$$

Here $\mathbf{z}^\rho = (z_1^\rho, \cdots, z_{d_1}^\rho)$, $\mathbf{z}^T = (z_1^T, \cdots, z_{d_1}^T)$, and $\mathbf{z}^b = z_1^b$ represent the random variables in the collision kernel, initial density and temperature.

space: 1d velocity: 2d random space: 15d

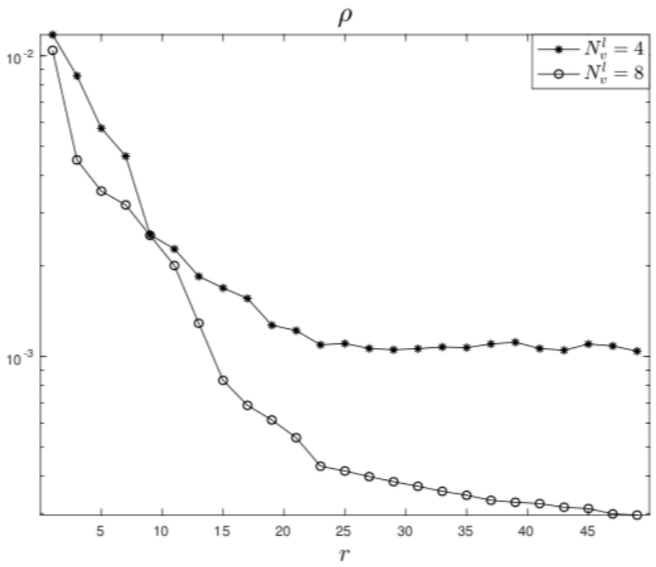
Fluid regimes

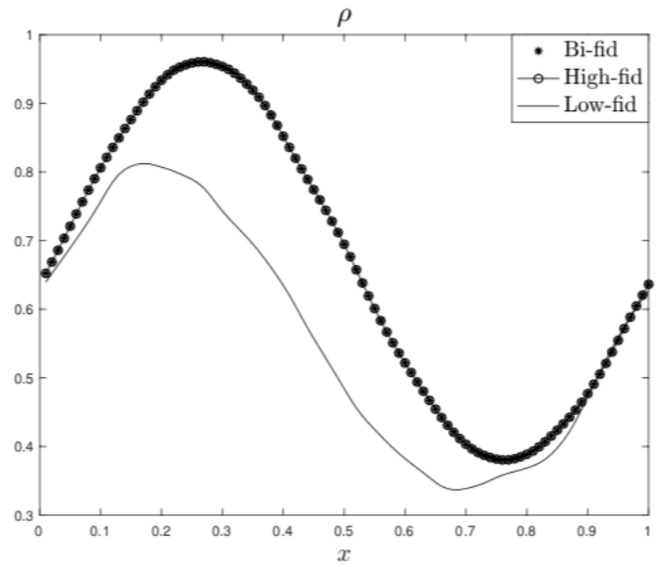


* The smaller Knudsen number is, the lower level errors saturate

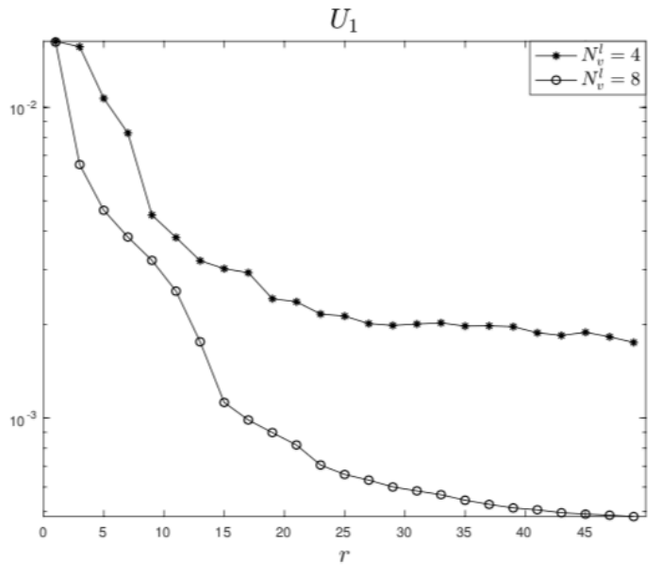
* As epsilon approaches to zero, the Euler (low-fid) commits *less modeling error,* thus can *capture more information* of the high-fid model.

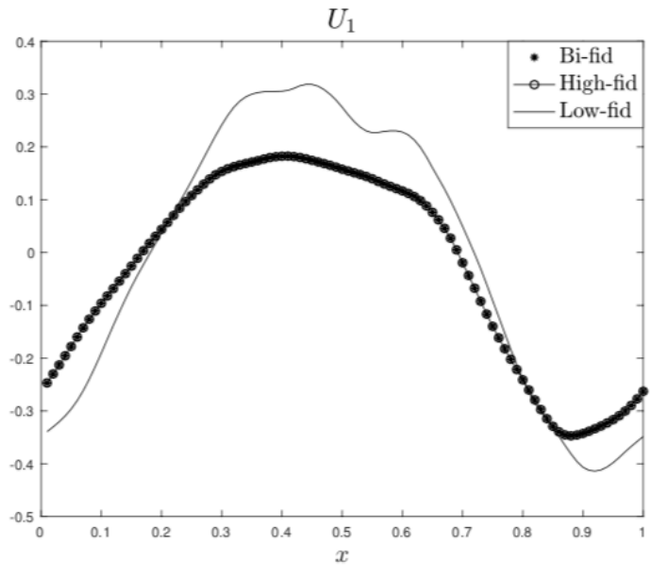
Kinetic regime $\varepsilon = 1$

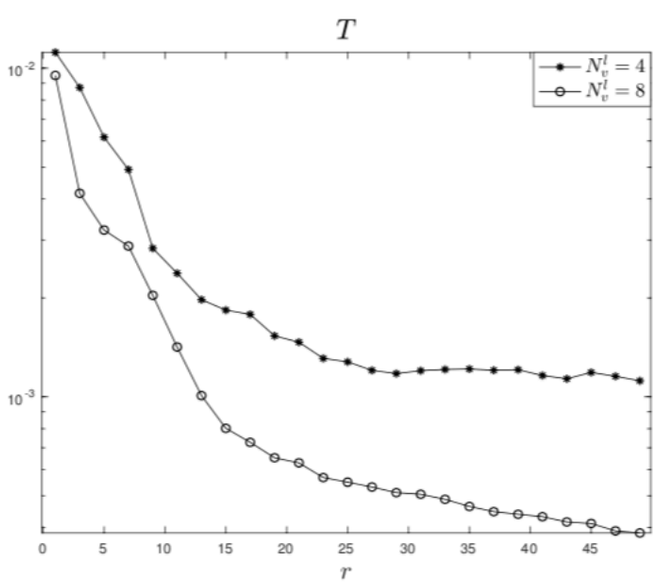


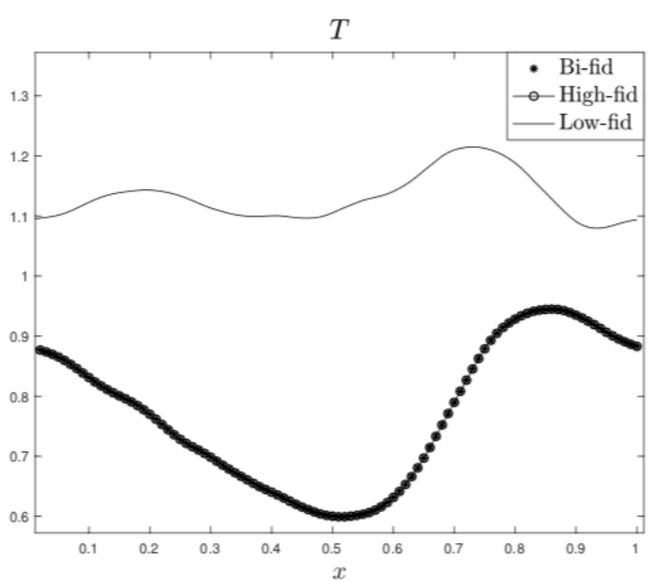


- The fluid description breaks down in the physical space, *yet* the BF approximation can still *capture important variations* of the high-fidelity model ***in the random space***









Example 2: Sod Shock Tube Test

* The collision kernel

$$b(\mathbf{z}^b) = 1 + 0.5 \sum_{k=1}^{d_1+1} \frac{z_k^b}{2k},$$

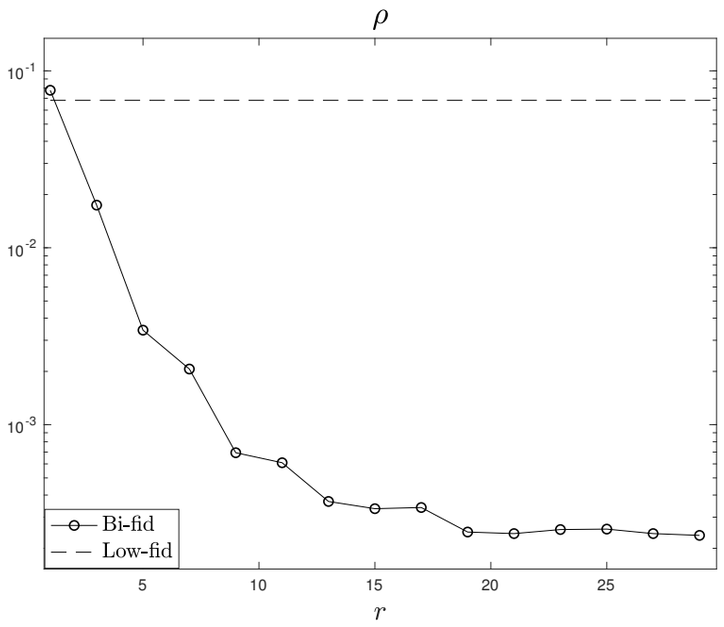
and the random initial distribution

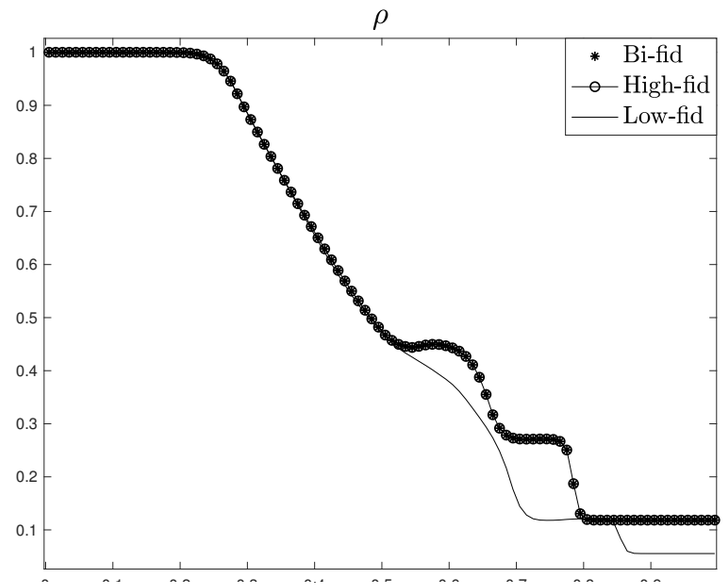
$$f^0(x, \mathbf{v}, \mathbf{z}) = \frac{\rho^0}{2\pi T^0} e^{-\frac{|\mathbf{v}-u^0|^2}{2T^0}},$$

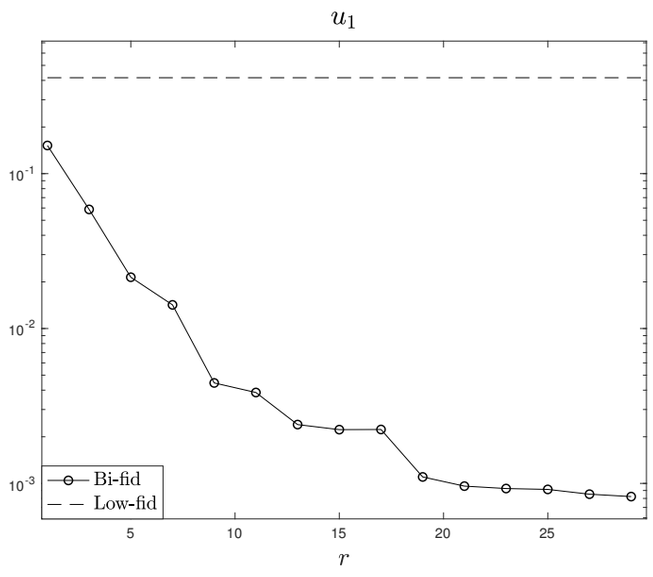
where the initial data for ρ^0, u^0 and T^0 is given by

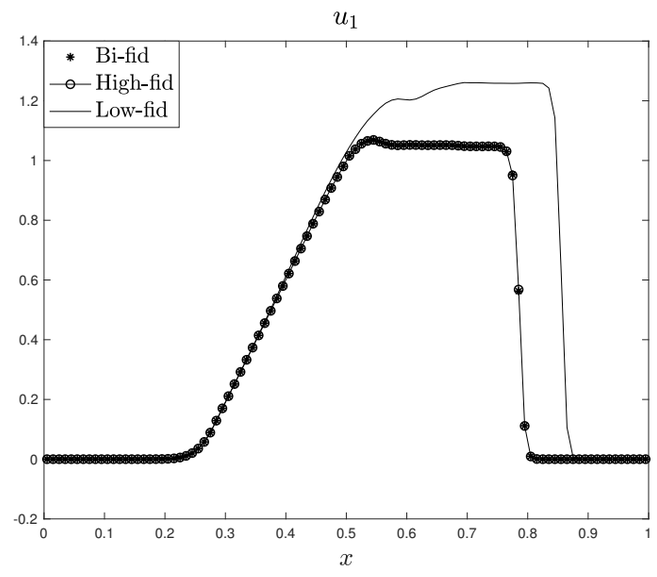
$$\begin{cases} \rho_l = 1, \qquad u_l = (0,0), \qquad T_l(\mathbf{z}^T) = 1 + 0.4 \sum_{k=1}^{d_1} \frac{z_k^T}{2k}, \qquad x \le 0.5, \\ \rho_r = \frac{1}{8}, \qquad u_r = (0,0), \qquad T_r(\mathbf{z}^T) = \frac{1}{8}(1 + 0.4 \sum_{k=1}^{d_1} \frac{z_k^T}{2k}), \qquad x > 0.5. \end{cases}$$

Fluid regime $\varepsilon = 10^{-4}$

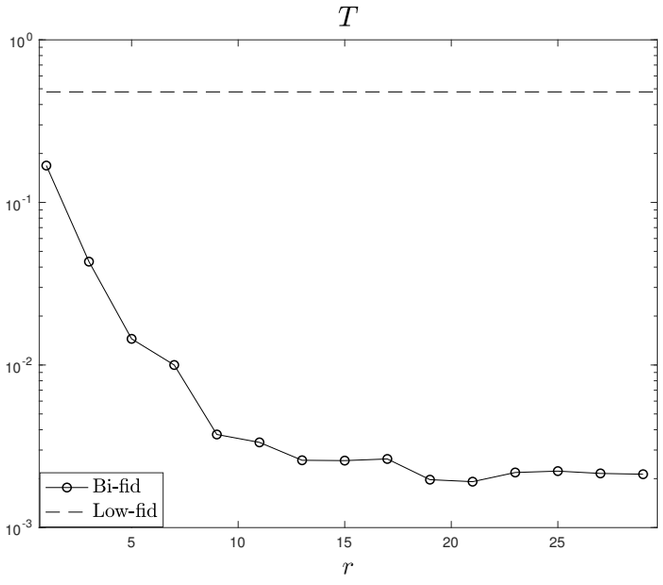


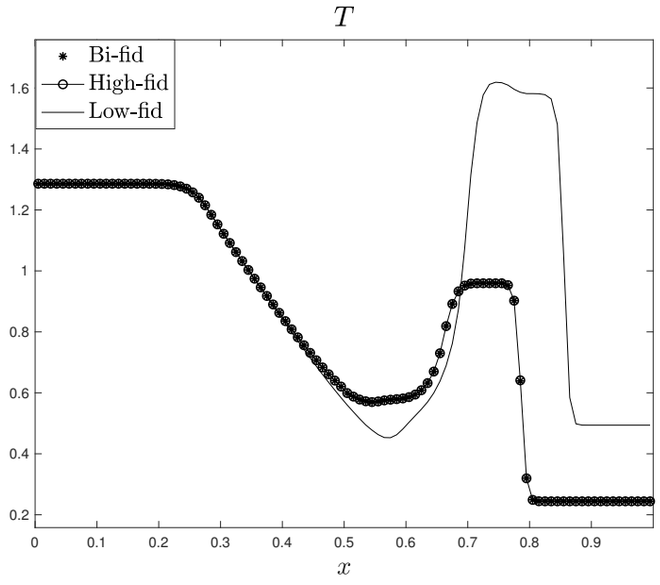






* 15-d random z needs only 10 high-fidelity (Boltzmann) runs!

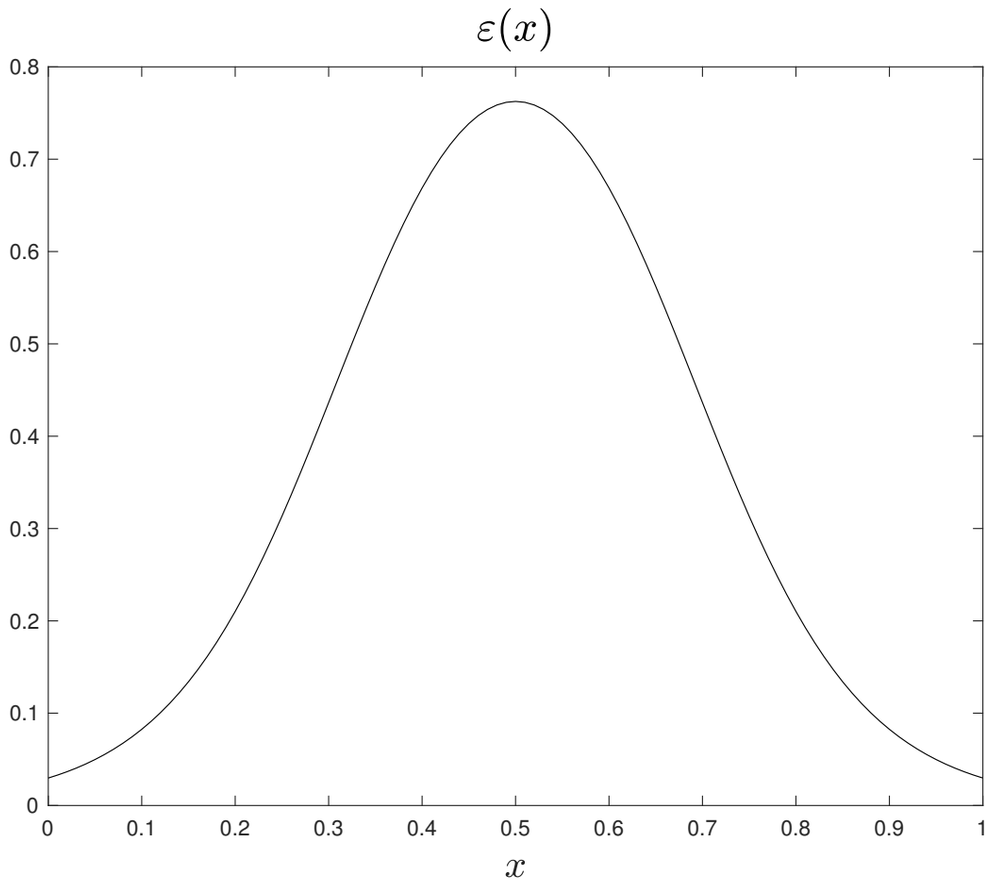




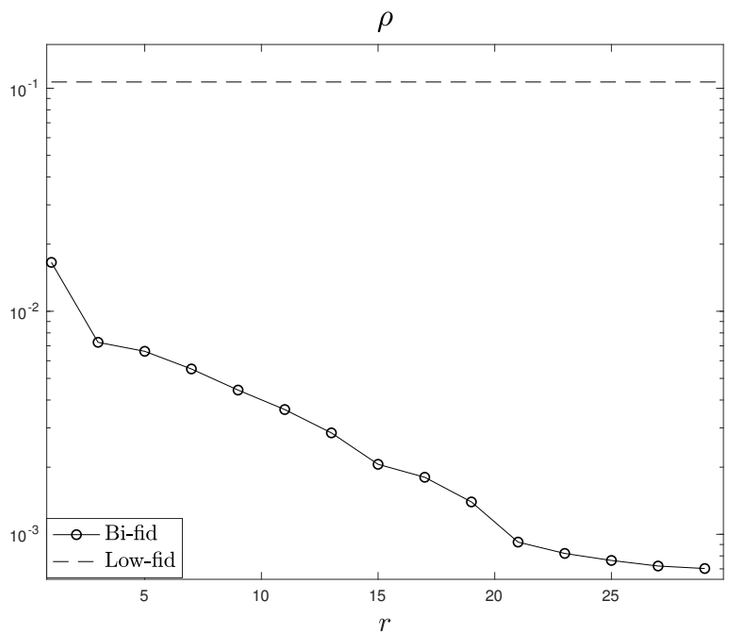
* Low-fid costs about **0.01** computation time of high-fid solver

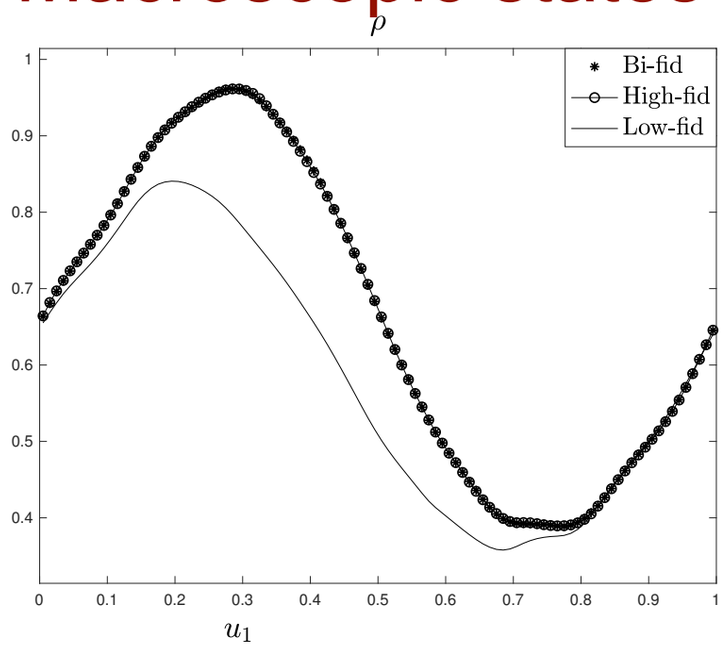
Example 3: Mixed regime

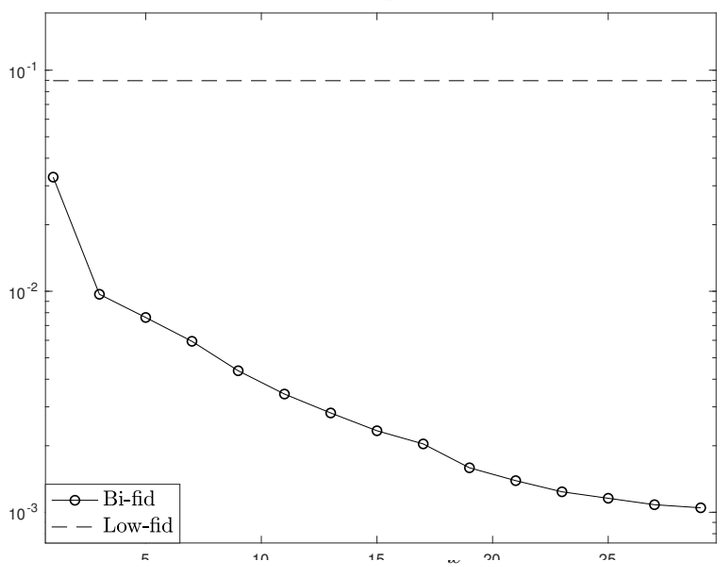
$$\varepsilon(x) = 10^{-3} + \frac{1}{2}\left[\tanh\left(1 - \frac{11}{2}(x - 0.5)\right) + \tanh\left(1 + \frac{11}{2}(x - 0.5)\right)\right]$$

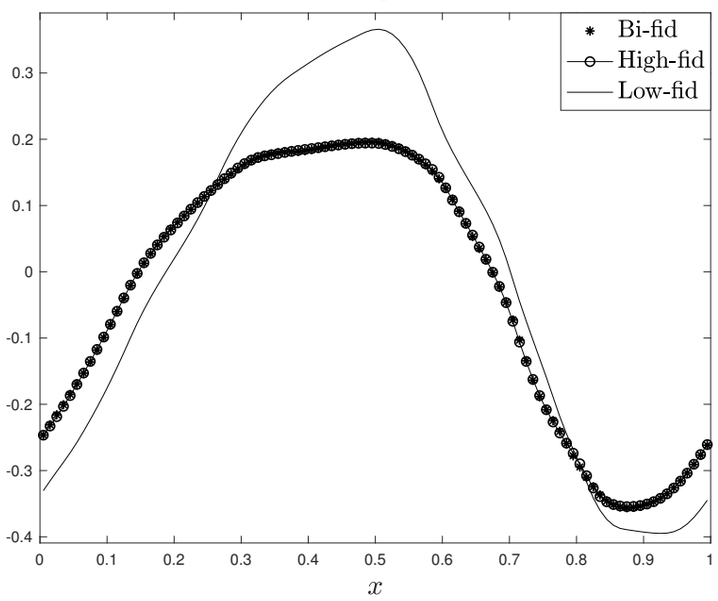


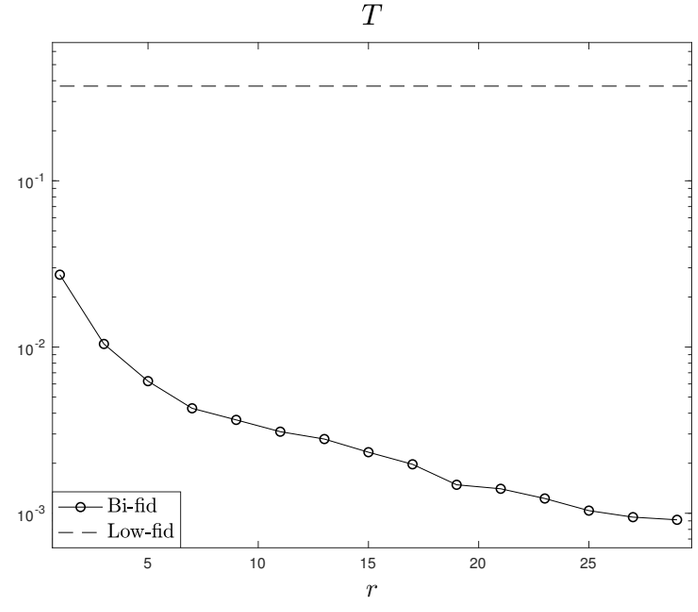
Macroscopic states

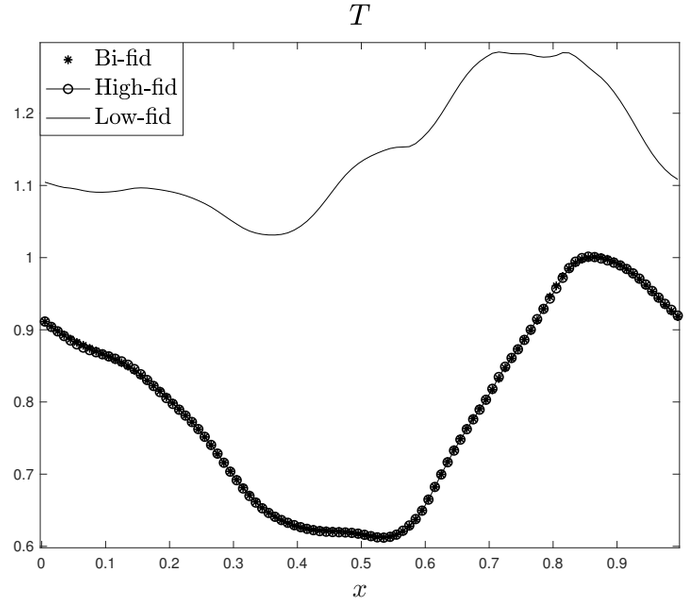












Bi-fidelity method for LTE

* Linear transport equation (LTE) under diffusive scaling:

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

* The Goldstein-Taylor (GT) model is:

$$\begin{cases} \partial_t u + \dfrac{1}{\varepsilon} \partial_x u = \dfrac{\sigma(x,z)}{2\varepsilon^2}(v-u), \\ \partial_t v - \dfrac{1}{\varepsilon} \partial_x v = \dfrac{\sigma(x,z)}{2\varepsilon^2}(u-v). \end{cases}$$

Let $\rho = u + v, \qquad s = \dfrac{u-v}{\varepsilon},$ then GT model becomes

$$\begin{cases} \partial_t \rho + \partial_x s = 0, \\ \partial_t s + \dfrac{1}{\varepsilon^2} \partial_x \rho = -\dfrac{\sigma(x,z)}{\varepsilon^2} s. \end{cases} \tag{3.2}$$

In the diffusion limit $\varepsilon \to 0$, system (3.2) can be approximated by the heat equation to the leading order, with random diffusion coefficient $\sigma(x,z)$:

$$\begin{cases} s = -\dfrac{1}{\sigma(x,z)} \partial_x \rho, \\ \partial_t \rho = \partial_x \left[\dfrac{1}{\sigma(x,z)} \partial_x \rho \right]. \end{cases} \tag{3.3}$$

* Liu-Pareschi-X.Zhu (21')

Bi-fidelity method for LTE

Motivations:

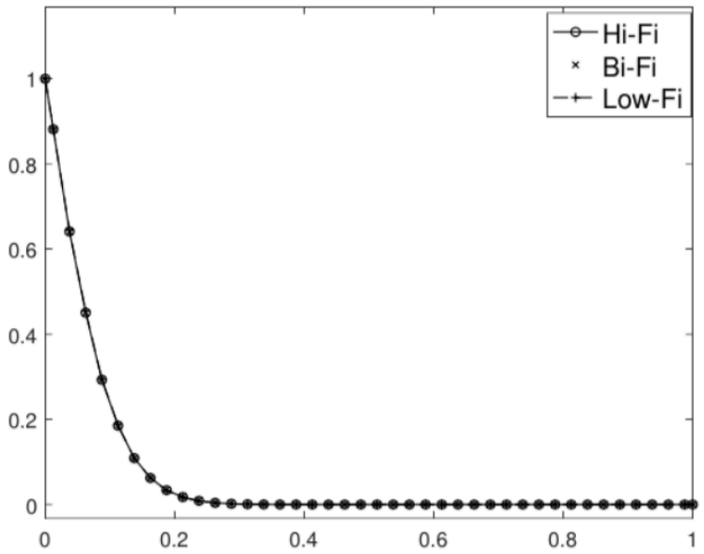
* We choose the GT equation as our low-fidelity model, which shares the same limiting diffusion equation as the LTE, by letting

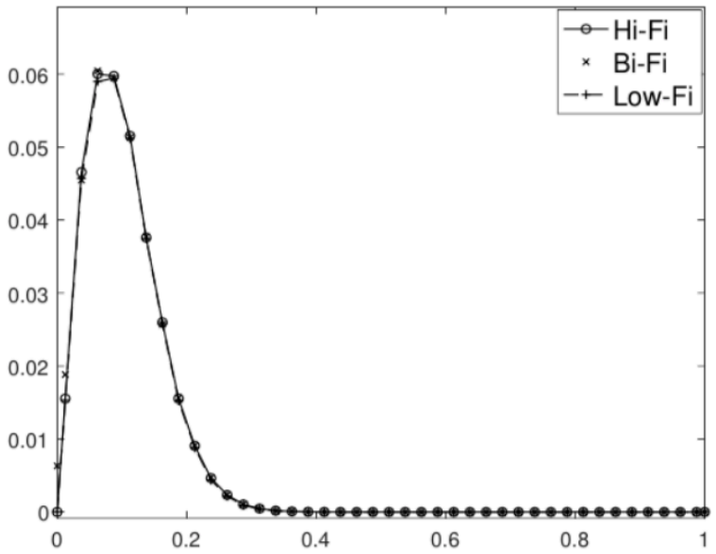
$$\sigma_{\mathrm{GT}} = \frac{1}{3}\sigma_{\mathrm{LTE}}$$

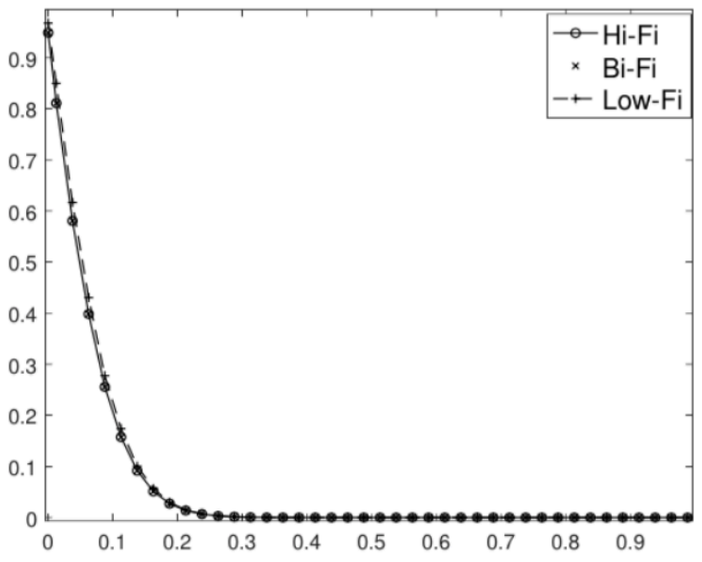
* Random cross section

$$\sigma(x,z) = 1 + \sigma \sum_{i=1}^{d} \frac{1}{(i\pi)^2} \cos(2\pi i x) z_i,$$

Bi-fidelity approximations







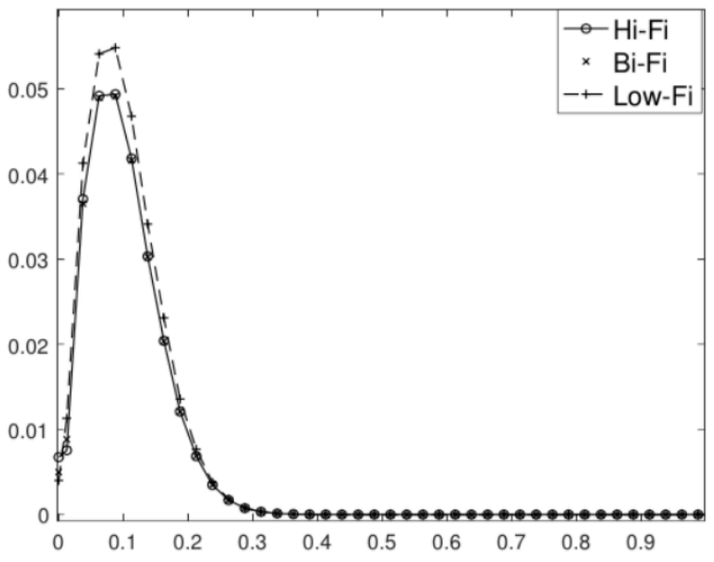


FIG. 5.1. *The mean (left) and standard deviation (right) of* $\overline{r}$ *at* $\varepsilon = 10^{-8}$ *(first row), and* $\varepsilon = 10^{-2}$ *(second row), obtained by* 12 *high-fidelity runs and the sparse grid method with* 2243 *quadrature points (crosses).*

Error plots

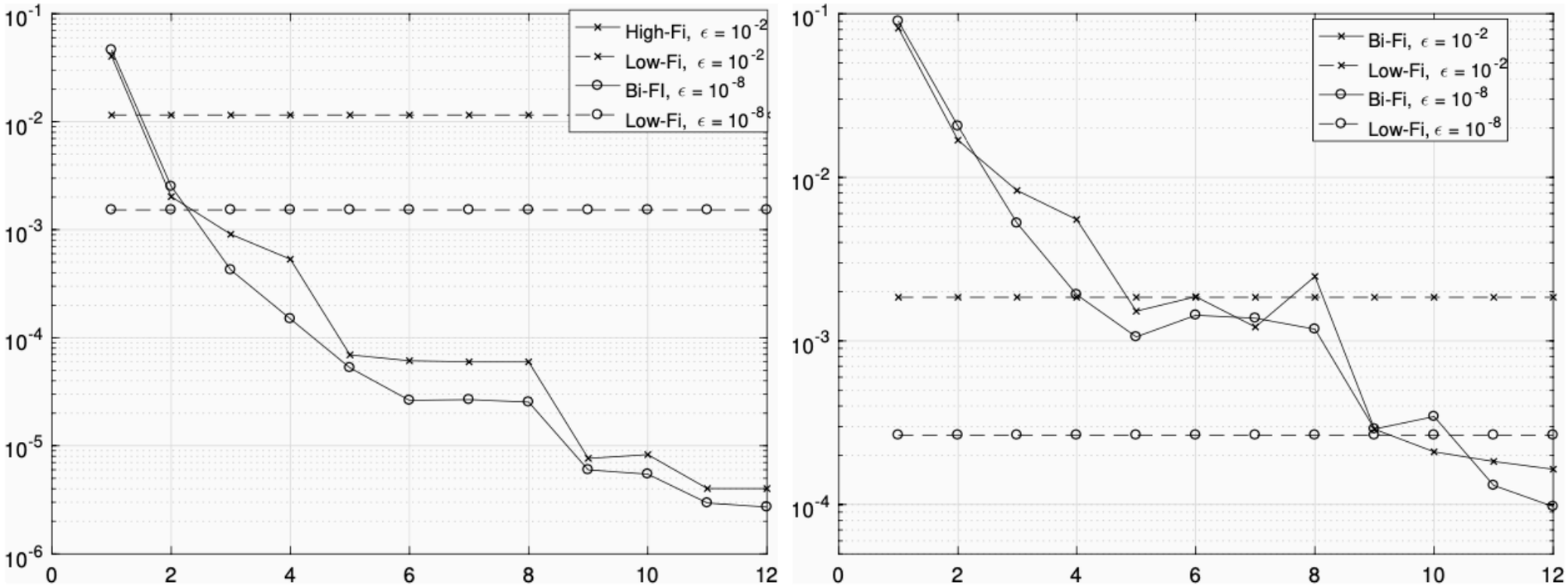


FIG. 5.3. *Errors of the bi-fidelity approximation mean (left) and standard deviation (right) of* $\overline{r}$ *for* $\epsilon = 10^{-8}$ *(circle)* , 10^{-2} *(cross) with respect to the number of high-fidelity runs, with* $d = 5$ *dimensional random input.*

* Fast convergence, high accuracy, with low computational cost

Numerical Examples

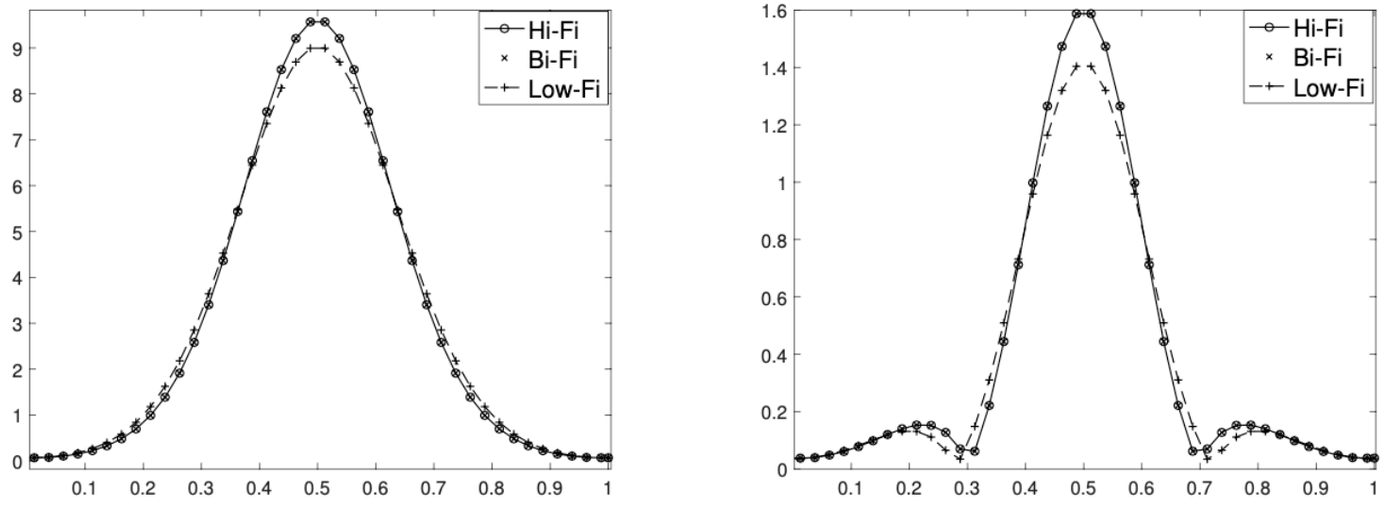


FIG. 6.10. *Test 4. The mean (left) and standard deviation (right) of $\overline{r}$, obtained by $r = 8$ high-fidelity runs and the sparse grid method with 2243 quadrature points (crosses).*

* A mixed regime test

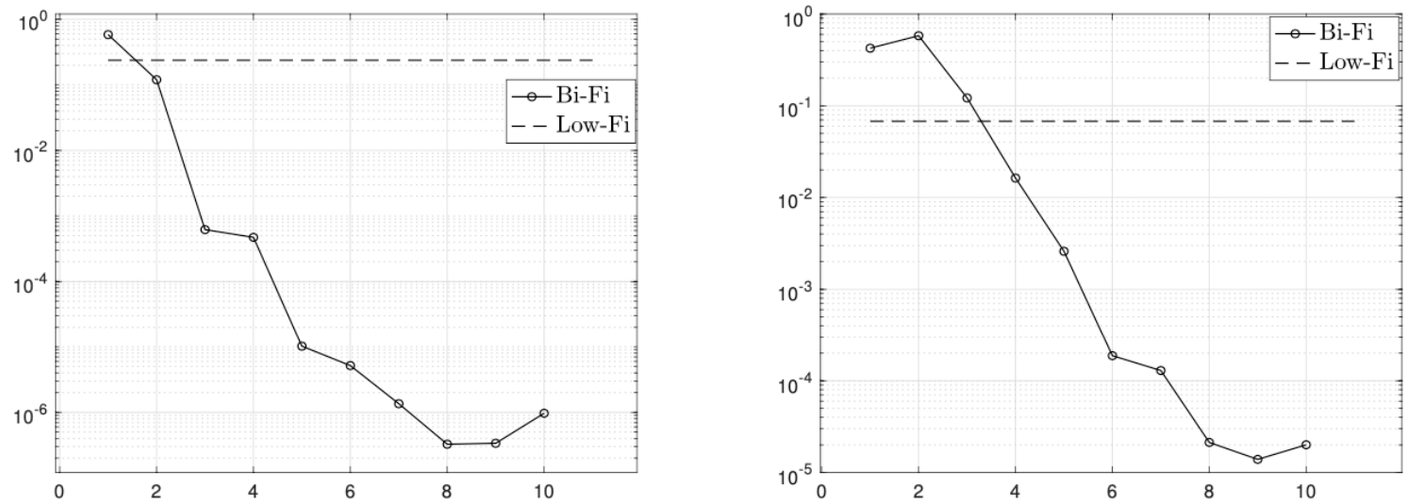


FIG. 6.11. *Test 4. Errors of the bi-fidelity approximation mean (left) and standard deviation (right) of $\overline{r}$ with respect to the number of high-fidelity runs.*

Hypocoercivity analysis

* *Hypocoercivity theory:* an important tool to study the stability and long-time behavior of the solution for kinetic equations

The study involves

(i) a *degenerate dissipative* kinetic operator;

(ii) a conservative operator $v \cdot \nabla_x$, such that the combination of these operators leads to a *convergence towards the global equilibrium state*;

and a Lyapunov functional (with mixed x, v derivatives) is needed to get a *quantitive* convergence rate.

* Many experts have contributed in this direction for deterministic models: Villani, Mouhot, Neumann, Guo, Duan, Briant, Arnold, Desvillettes, Dolbeault, Schmeiser, etc.

* Local parameter sensitivity analysis studies the long-time behavior of the solution; explore how the randomness of the "input" propagates in time and how it affects the solution in the long time.

Sensitivity analysis for the analytic solution

Main results:

If the initial data and collision kernel are random (under suitable assumptions), we have the following results on the convergence to global equilibrium:

(i) Under the incompressible Navier-Stokes scaling,

$$||h||_{H^{s,r}_{x,v}L^\infty_z} \le C_I\, e^{-\tau_s t}, \qquad ||h||_{H^s_{x,v}H^r_z} \le C_I\, e^{-\tau_s t}.$$

(ii) Under the acoustic scaling,

$$||h||_{H^{s,r}_{x,v}L^\infty_z} \le C_I\, e^{-\varepsilon\tau_s t}, \qquad ||h||_{H^s_{x,v}H^r_z} \le C_I\, e^{-\varepsilon\tau_s t},$$

where C_I, τ_s are positive constants independent of ε.

* Liu-Jin (SIAM MMS 18')
* E.Daus-Jin-Liu (KRM 19'): improvement on the assumptions for random collision kernel

Error analysis for bi-fidelity method

* In Gamba-Jin-Liu 19', we use projection error of the *greedy algorithm* (Cohen-DeVore, 15') and adapt the hypocoercivity analysis to conduct error analysis of bi-fidelity method for a general class of multiscale kinetic problems.

* Splitting the error:

$$
\begin{aligned}
& u^H(z) - u^B(z) \\
&= u^H(z) - \sum_{n=1}^{N} c_n(z)\, u^H(z_n) \\
&= u^H(z) - u^L(z) + \left(u^L(z) - \sum_{n=1}^{N} c_n(z)\, u^L(z_n) \right) + \sum_{n=1}^{N} c_n(z) \left(u^L(z_n) - u^H(z_n) \right).
\end{aligned}
$$

Perturbative setting: $f = \mathcal{M} + \delta M h$

↓

small

Error analysis for bi-fidelity method

Under reasonable assumptions for the random collision kernel, if the initial data satisfies

$$||h_{in}||_{H^s_{x,v}L^\infty_z} \leq \frac{\varepsilon}{\delta}\eta_s,$$

with η_s sufficiently small, then for all $t > 0$,

$$\|u^H(t) - u^B(t)\|_{H^s_x L^2_z} \leq \frac{C_1}{(N/2+1)^{q/2}} + C_2\,\delta,$$

where N is the number of high-fidelity simulation runs.

* error *decays algebraically* with respect to N
* convergence rate *independent of* the dimension of the random space
* *uniform* in the Knudsen number estimate
* error estimate valid in both kinetic and hydrodynamic regimes

Other relevant work in the multi-fidelity framework

* Dimarco-Pareschi (19',20') on multiscale control variate methods, Hu-Pareschi-Wang (20') on MLMC method for the BGK model;

* Multi-fidelity moment method for the BGK model with uncertainties (with Wang-Li-Liang-Zhu 21'), …..

Conclusions

* Bi-fidelity stochastic collocation method *accelerate the computation* of multiscale kinetic equations with high-dimensional random parameters;

* The hypocoercivity analysis for multiscale kinetic problems with uncertainty provides a tool to conduct *error analysis* for the bi-fidelity method;

* practical error bound, etc.

Future work:

* build *a hierarchy of fidelity models*
* extend to higher dimensions with more complex random variables and collision kernels
* study sharper error estimates for control variate variance reduction MLMC method
* study kinetic equations using deep learning approaches (Chen-Liu-Mu 21', Liu-Zhang-Zeng 21'), etc.

Thank you for your attention!