# To Understand Uncertainty Quantification

XIAO Tianbai

# What's UQ?

Combining computational models, physical observations, and possibly expert judgment to make inferences about a physical system.

**David Higdon,** Los Alamos National Lab

Uncertainty quantification attempts to express the known unknowns.

**Bill Oberkampf,** Sandia National Lab

UQ is about providing bounds on our knowledge of system behavior and on confidence in our predictions.

**Omar Knio,** Johns Hopkins University

UQ is the difference between success and failure.

**Gianluca** Iaccarino, Stanford University

# What’s UQ?

UQ is quantification of the effect of uncertainty. It sounds boring indeed but I don't see anything else to it.
**Dongbin Xiu,** Purdue University

Man – that’s a hard question!!
**Tim Trucano,** Sandia National Lab

Counting sh*t you can’t see.
**Carter Rose,** Dallas, Texas

# What’s UQ?

I guess “uncertainty" means a lack of certainty or knowledge; i.e. ignorance. This is one definition that suggests that subjective probability may be a reasonable way to think of uncertainty wherein randomness refers to a lack of knowledge. Quantification, of course, means to quantify, to observe and assign a measure. I like the Wikipedia definition: an act of measuring that maps human observations and experiences into a set of numbers. I would weaken that a little: human observations include those made by humans using instruments. Thus, Uncertainty Quantifivation is precisely the **quantification of one's lack of knowledge concerning (in science and engineering) a physical reality**.

**J. Tinsley Oden,** The University of Texas at Austin

# UQ in CFD

Cauchy problem for the scalar conservation law

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla_x \cdot \mathbf{F}(\mathbf{U}) = \mathbf{0}, t > 0$$

$$\mathbf{U}(\mathbf{x}, 0) = \mathbf{U}_0(\mathbf{x}), \mathbf{x} \in \mathbb{R}^d$$

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla_x \cdot \mathbf{F}(\mathbf{U}, \omega) = \mathbf{0}, t > 0$$

**Randomness** could come from

- random flux coefficients $\omega$
- the initial data $U^0(x,z)$
- the boundary data $U^b(t,x,z)$

# Stochastic Sod Problem with Random Initial Data

Riemann problem for the Euler equations

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U})}{\partial x} = \mathbf{0}, \quad x \in (0,2)$$

$$\mathbf{U}(x,0,y) = \mathbf{U}_0(x,y) = \begin{cases} \mathbf{U}_L, x < Y(\omega) \\ \mathbf{U}_R, x > Y(\omega) \end{cases}$$

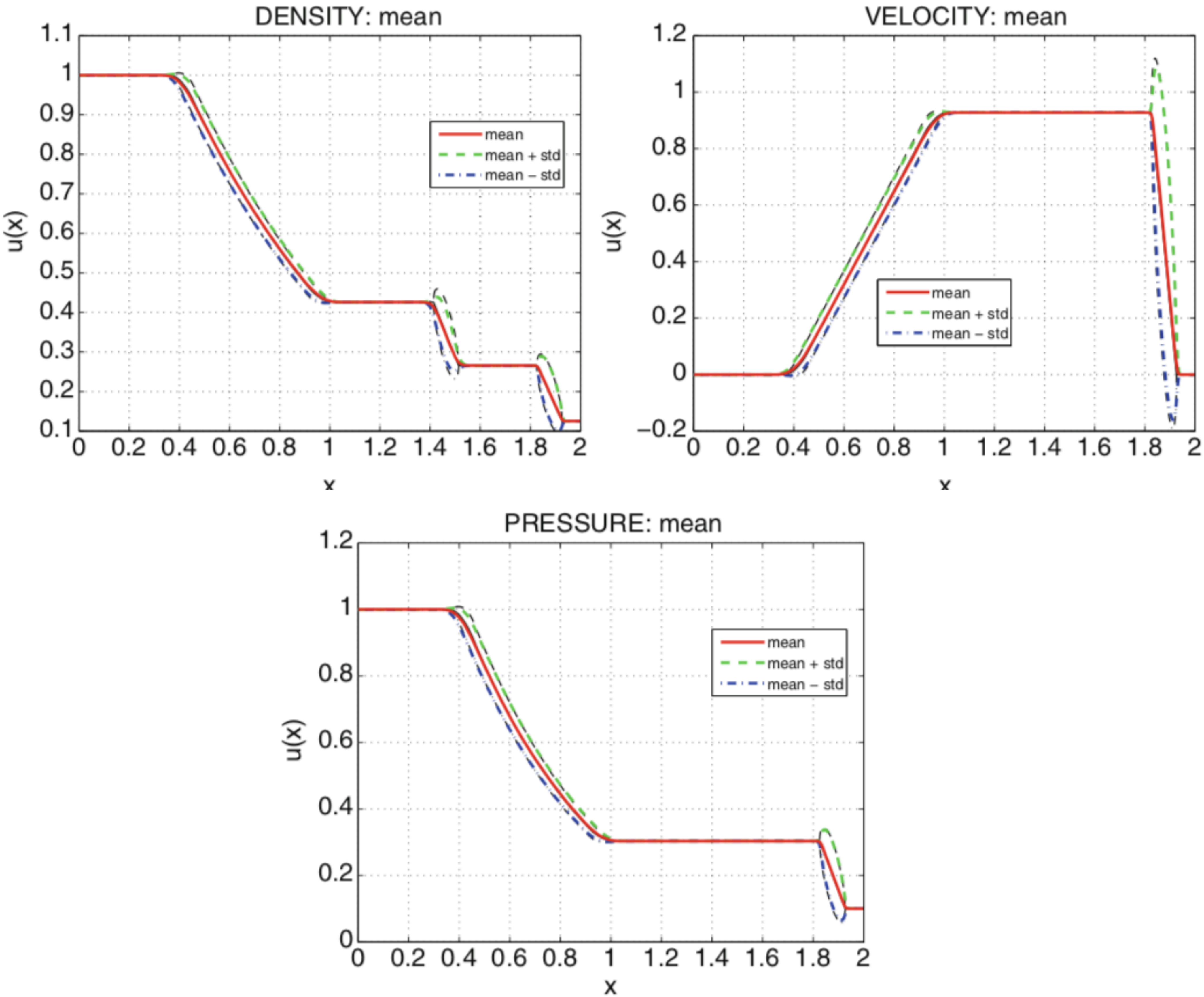
$$y = Y(\omega), \omega \in \Omega$$

Apply the SFV method to solve the system with Y(\omega) uniformly distributed on [0.95; 1.05]

$$\mathbf{W}_0(x,\omega) = [\rho_0(x,\omega), u_0(x,\omega), p_0(x,\omega)]^\top = \begin{cases} [1.0, 0.0, 1.0] & \text{if } x < Y(\omega) \\ [0.125, 0.0, 0.1] & \text{if } x > Y(\omega) \end{cases}$$


[1] Schwartzentruber, T. E., and Boyd, I. D. (2006). A hybrid particle-continuum method applied to shock waves. Journal of Computational Physics, 215(2), 402-416.
[2] Filbet, F., and Jin, S. (2010). A class of asymptotic-preserving schemes for kinetic equations and related problems with stiff sources. Journal of Computational Physics, 229(20), 7625-7648.

# Stochastic Sod Problem with Random Initial Data



# Stochastic Sod Problem with Random Initial Data and Flux

Riemann problem for the Euler equations

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}(\mathbf{U},\omega)}{\partial x} = \mathbf{0}, \quad x \in (0,2)$$

$$\mathbf{U}(x,0,\omega) = \mathbf{U}_0\left(x, Y_1(\omega), Y_2(\omega)\right) = \begin{cases} \mathbf{U}_L\left(Y_2(\omega)\right), x < Y_1(\omega) \\ \mathbf{U}_R, x > Y_1(\omega) \end{cases}$$

$$\mathbf{U} = [\rho, \rho u, E]^\top, \mathbf{F} = \left[\rho u, \rho u^2 + p, \rho u(E+p)\right]^\top$$

$$\mathbf{F}(\mathbf{U},\omega) = \mathbf{F}\left(\mathbf{U}, Y_3(\omega)\right) \qquad p = (\gamma - 1)\left(E - \tfrac{1}{2}\rho u^2\right)$$

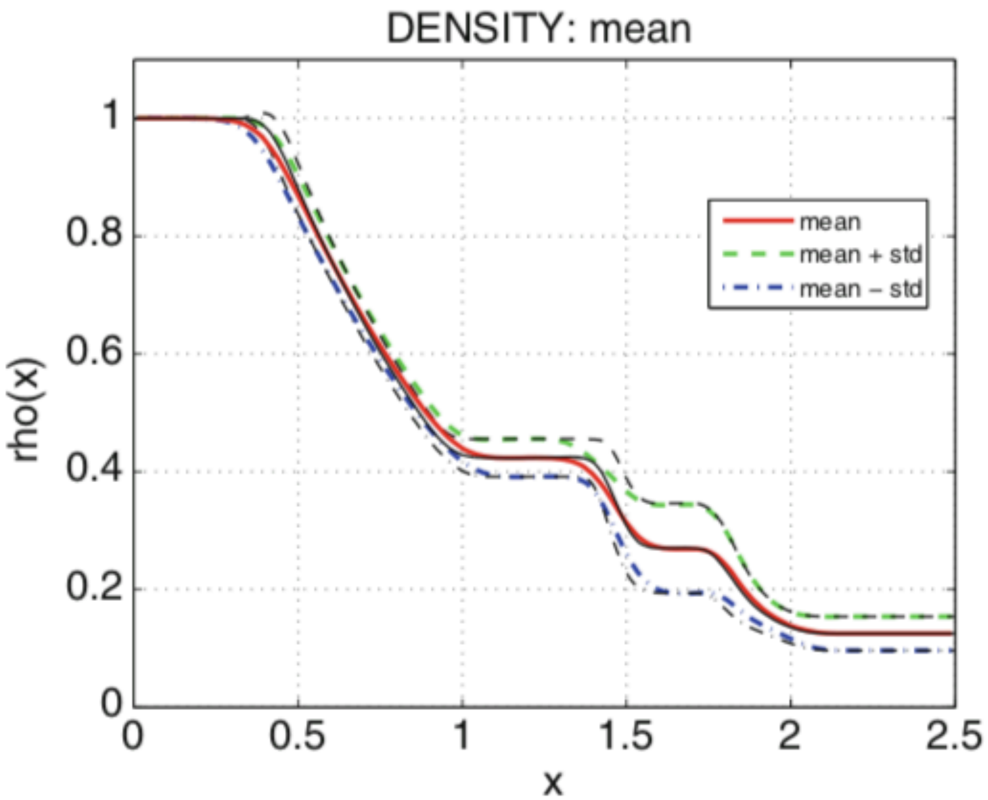
$$\gamma = \gamma\left(Y_3(\omega)\right)$$

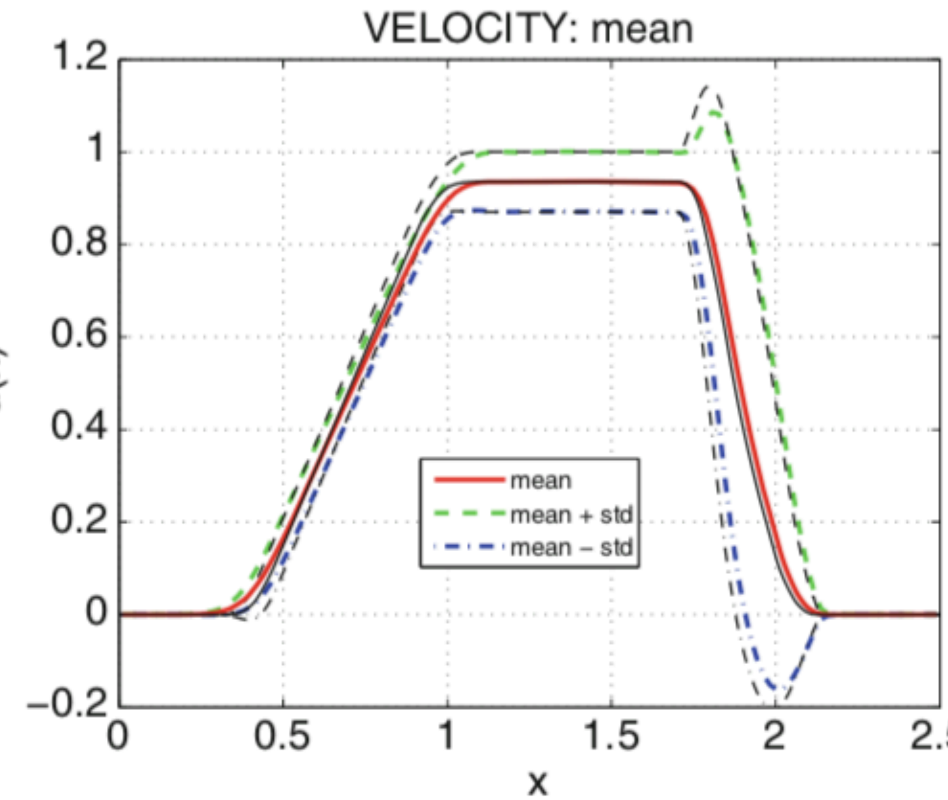
$$\mathbf{W}_0(x,\omega) = [\rho_0(x,\omega), u_0(x,\omega), p_0(x,\omega)]^\top$$

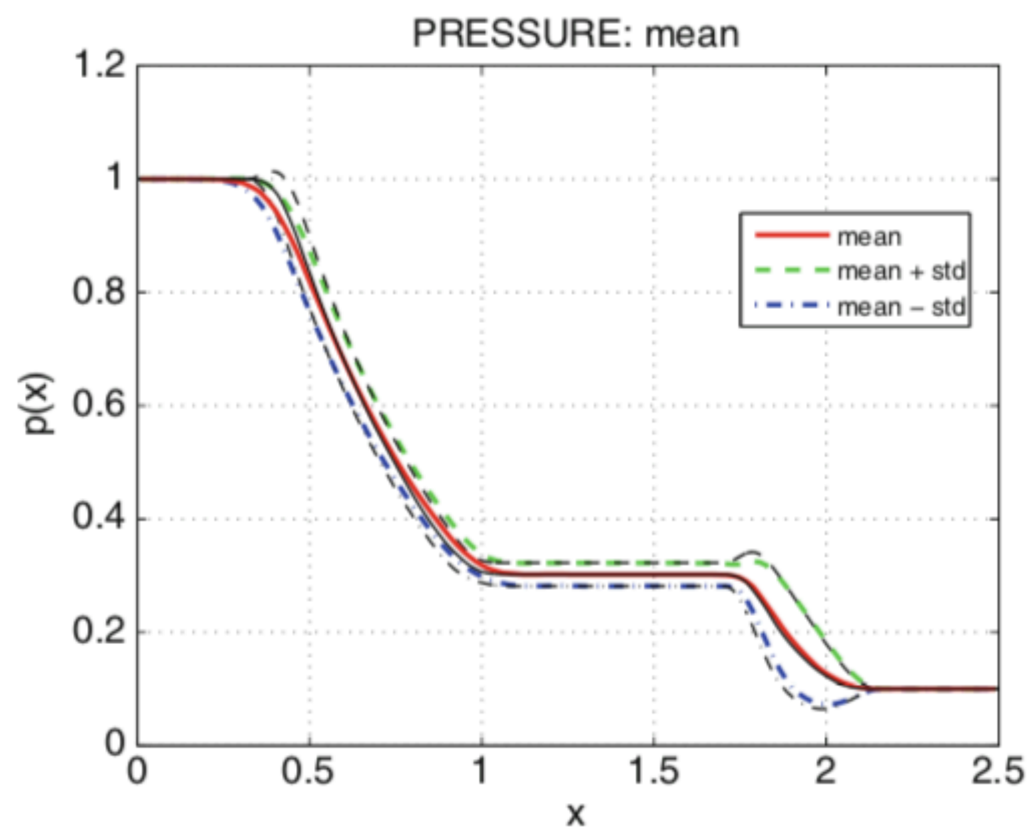
$$\begin{aligned} &= [1.0, 0.0, 1.0] && x < Y_1(\omega) \\ &\quad [0.125 + 0.5Y_2, 0.0, 0.1] && x > Y_1(\omega) \end{aligned}$$

Y1~U[0.95,1.05], Y2~U[0.1,0.1], Y3~U[1.2,1.6]

# Stochastic Sod Problem with Random Initial Data and Flux



# UQ in kinetic theory: plus collision effect

Cauchy problem for the kinetic equation

$$\begin{cases} \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\mathrm{Kn}} \mathcal{Q}(f,f)(t,\mathbf{x},\mathbf{v},\mathbf{z}), & t > 0, \mathbf{x} \in \Omega, \mathbf{v} \in \mathbb{R}^d, \mathbf{z} \in I_{\mathbf{z}} \\ f(0,\mathbf{x},\mathbf{v},\mathbf{z}) = f^0(\mathbf{x},\mathbf{v},\mathbf{z}), & \mathbf{x} \in \Omega, \mathbf{v} \in \mathbb{R}^d, \mathbf{z} \in I_{\mathbf{z}} \\ f(t,\mathbf{x},\mathbf{v},\mathbf{z}) = g(t,\mathbf{x},\mathbf{v},\mathbf{z}), & t \geq 0, \mathbf{x} \in \partial\Omega, \mathbf{v} \in \mathbb{R}^d, \mathbf{z} \in I_{\mathbf{z}} \end{cases}$$

**Randomness** could come from

- the collision kernel, for instance, $B = b_\lambda(z^B)|v - v_*|^\lambda$;
- the boundary data g(t,x,v,z), in which $u_w$ and Tw are replaced by $u_w(t,x,z^b)$ and $T_w(t,x,z^b)$;
- the initial data $f^0(x,v,z)$, via initial macroscopic quantities: density $\rho 0(x,z^i)$, temperature $T0(x,z^i)$, etc.

# UQ in kinetic theory: plus collision effect

numerical methods developed for uncertainty quantification

- Monte Carlo methods: sample randomly in the random space, which results in halfth order convergence

- stochastic collocation methods: use sample points on a well-designed grid, and one can evaluate the statistical moments by numerical quadratures.

- stochastic Galerkin methods: start from an orthonormal basis in the random space, and approximate functions by truncated polynomial chaos expansions.

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

$$< \Phi_{\mathbf{k}}, \Phi_{\mathbf{j}} >_\omega = \int_{l_k} \Phi_{\mathbf{k}}(\mathbf{z})\Phi_{\mathbf{j}}(\mathbf{z})\omega(\mathbf{z})\mathrm{d}\mathbf{z} = \delta_{\mathbf{k},}, \quad 0 \le |\mathbf{k}|, |\mathbf{j}| \le M$$

# Stochastic Boltzmann solution

Homogeneous relaxation with random collision kernel

$$\frac{\partial f}{\partial t} = B(\mathbf{z})(\mathcal{M} - f)$$

or Boltzmann collision operator, with

$$f^0(v) = v^2 e^{-v^2}$$

$$B(\mathbf{z}) = 1 + s_1 z_1 + s_2 z_2, \quad s_1 = 0.2, s_2 = 0.1$$

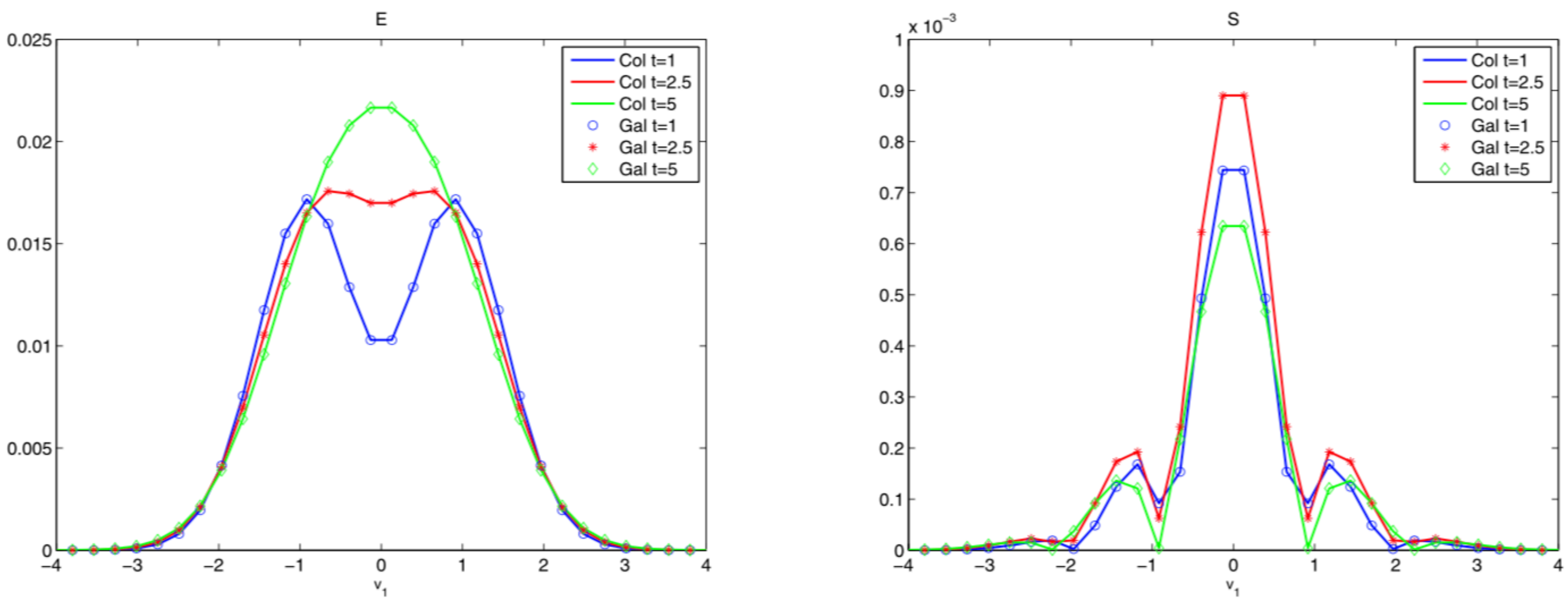



**Fig. 4.** Example 2. $\mathbb{E}[f]$ and $S[f]$ at $v_2 = 0$. "Col" stands for collocation, "Gal" stands for Galerkin. Heun is used for Galerkin, RK-4 is used for collocation.