To Understand Uncertainty Quantification

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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, Ohio State 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**.

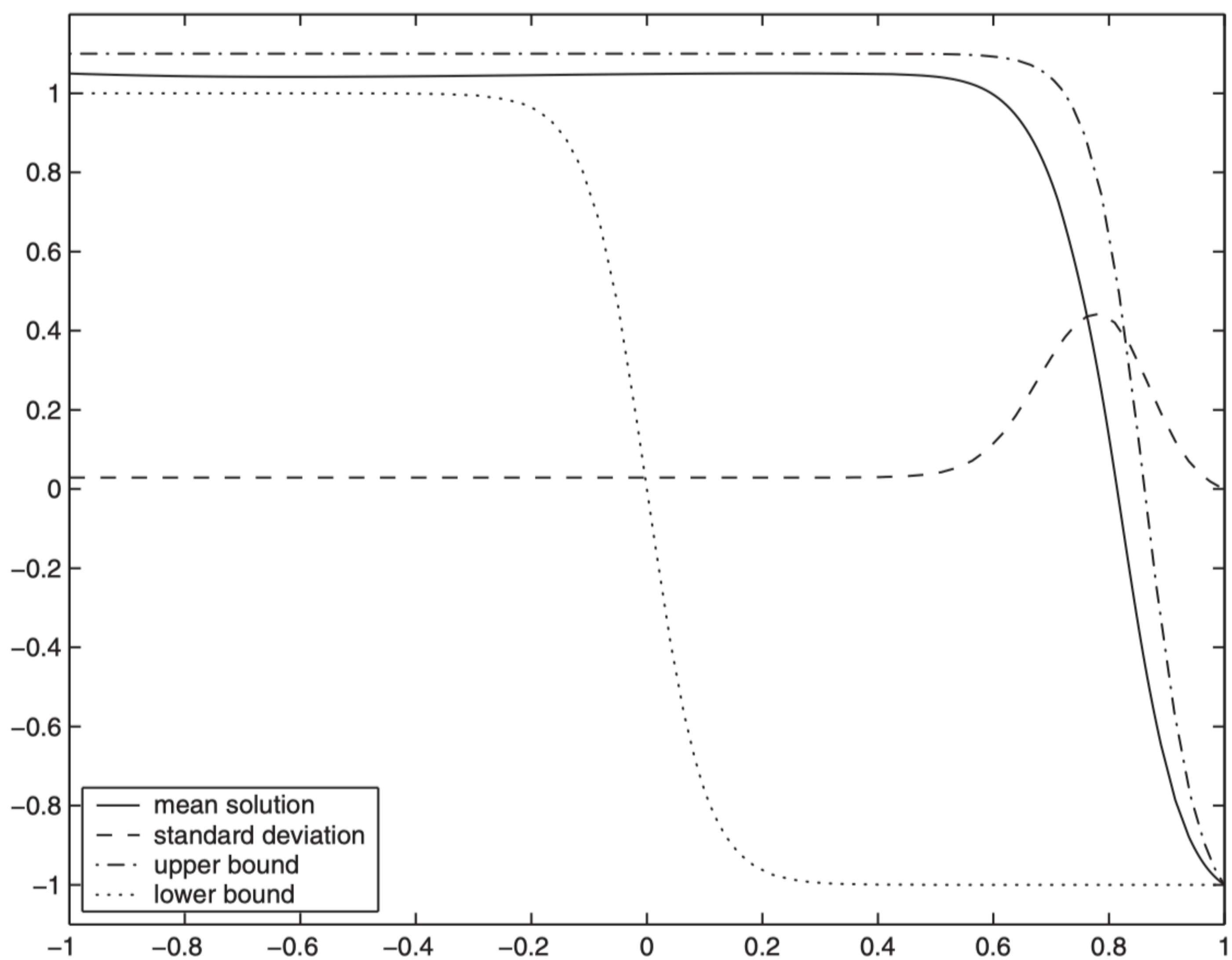
J. Tinsley Oden, The University of Texas at Austin

An illustrative example of UQ: Burgers' Equation

Viscous Burgers' equation

$$\begin{cases} u_t + uu_x = vu_{xx}, & x \in (-1,1) \\ u(-1) = 1, & u(1) = -1 \end{cases}$$

$$u(-1,t) = 1 + \delta$$



UQ in CFD

Cauchy problem for hyperbolic 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 ω
- 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

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

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

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

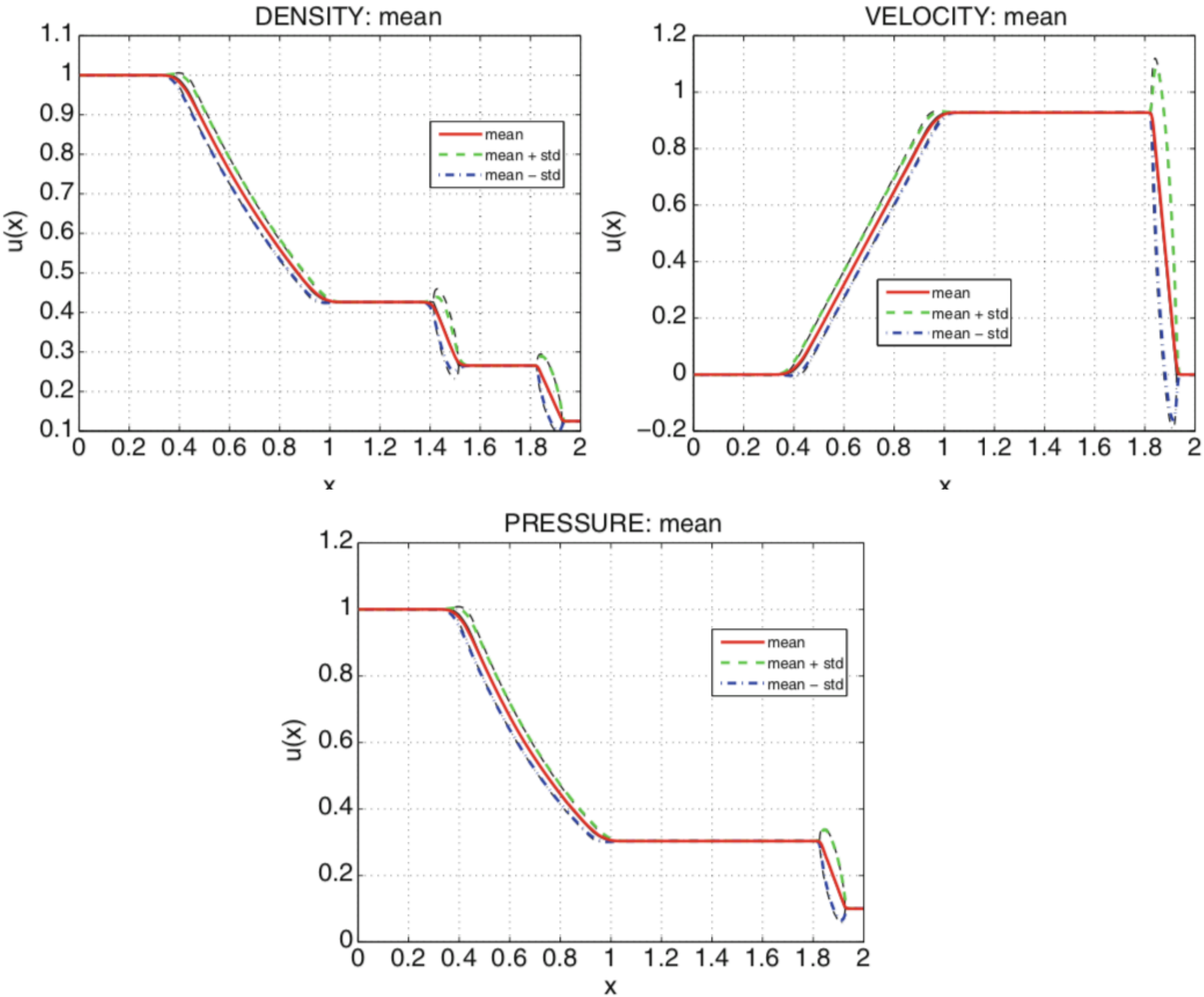
Apply the SFV method to solve the system with Y(\omega) uniformly distributed on [0.95; 1.05]

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

[1] Schwab, C., and Tokareva, S. (2013). High order approximation of probabilistic shock profiles in hyperbolic conservation laws with uncertain initial data∗∗∗. *ESAIM: Mathematical Modelling and Numerical Analysis*, *47*(3), 807-835.

[2] Abgrall, R., and Tokareva, S. (2017). The Stochastic Finite Volume Method. In *Uncertainty Quantification for Hyperbolic and Kinetic Equations* (pp. 1-57). Springer, Cham.

Stochastic Sod Problem with Random Initial Data



Stochastic Sod Problem with Random Initial Data and Flux

Riemann problem for the Euler equations

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

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

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

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

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

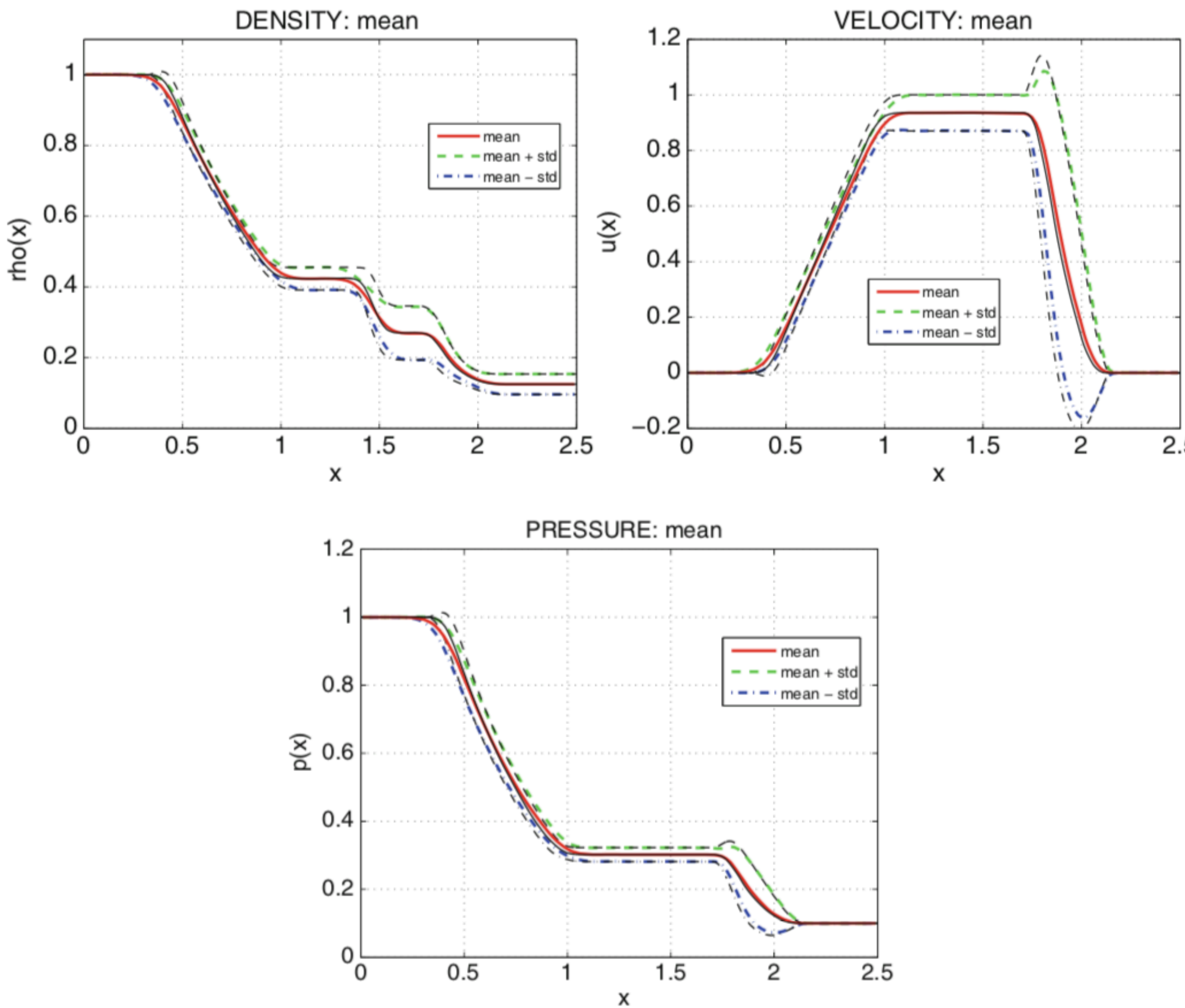
$$\mathbf{W}_0(x,\omega) = [\rho_0(x,\omega), u_0(x,\omega), p_0(x,\omega)]^\top$$

$$= [1.0, 0.0, 1.0] \qquad x < Y_1(\omega)$$

$$[0.125 + 0.5Y_2, 0.0, 0.1] \qquad x > Y_1(\omega)$$

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

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

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

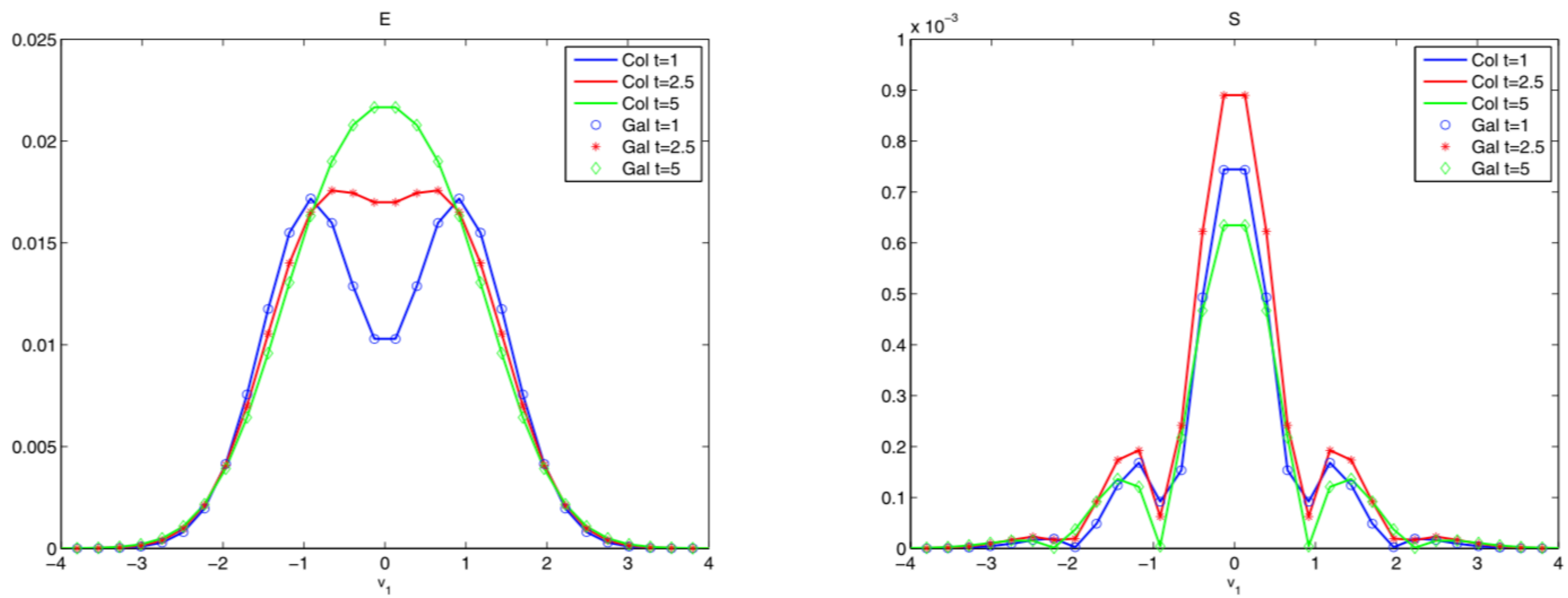


Fig. 4. Example 2. $\mathbb{E}[f]$ and $S[f]$ at $v_2 = 0$. "Col" stands for collocation, "Gal" stands for Galerkin. Heun is used for Galerkin, RK-4 is used for collocation.

Stochastic Boltzmann solution

Other scenarios

Random initial data, e.g.

$$\begin{cases} \rho_l = 1 + s_1 \left(\dfrac{z+1}{2}\right), \quad u_l = 0, \quad T_l = 1 + s_2 z, \quad x \leq 0.5, \\ \rho_r = 0.125, \quad u_r = 0, \quad T_r = 0.25, \quad x > 0.5. \end{cases}$$

Random boundary data, e.g.

$$T_W(z) = 2(T_0 + sz), \quad s = 0.2.$$