

PDF Methods for Uncertainty Quantification in Hyperbolic Conservation Laws

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Abstract

We developed a probabilistic method to quantify uncertainty associated with hyperbolic conservation laws. The approach relies on the concept of fine-grained probability density function (PDF) or cumulative density function (CDF) and derives a deterministic equation for the PDF/CDF of the system state. It is computationally efficient and enables one to obtain full statistical description of system states, which is necessary for risk assessment. We demonstrate three such examples, namely, advection-reaction equation, kinematic wave equation and advective-diffusive transport, respectively.

Hyperbolic conservation laws

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{f}(c; \mathbf{x}, t) = r(c; \mathbf{x}, t)$$

PDF Methods for Parametric Uncertainty

- Deterministic PDE of system states PDFs
- No linearization of SPDEs
- Complete statistics of system states
- Computationally efficient and accurate

Raw Distribution:

$$\Pi(c, C; x, t) = \delta[C - c(x, t)]$$

Probability Density Function (PDF):

$$\bar{\Pi}(c, C; x, t) = p_c(C; x, t)$$

Advective-Reactive Transport

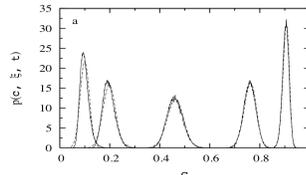
$$\frac{\partial c}{\partial t} = -\nabla \cdot (\mathbf{u}c) + \alpha f_\alpha(c), \quad f_\alpha = -k(c^\alpha - C_{eq}^\alpha)$$

Sources of Uncertainty:

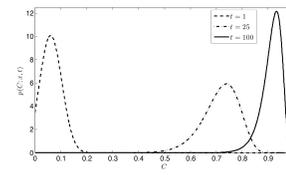
Velocity field $u(x, t, \omega)$ & Reaction rate $k(x, \omega)$

PDF Equation:

$$\frac{\partial p_c}{\partial t} = -\frac{\partial \tilde{u}_i p_c}{\partial \tilde{x}_i} + \frac{\partial}{\partial \tilde{x}_k} \left[\tilde{D}_{ij} \frac{\partial p_c}{\partial \tilde{x}_i} \right], \quad \left\{ \begin{array}{l} \tilde{\mathbf{x}} = (x_1, x_2, x_3, C)^T \\ \tilde{\mathbf{u}} = (u_1, u_2, u_3, f_\alpha)^T \end{array} \right.$$



Temporal evolution of the concentration PDF with deterministic velocity at increasing times (from left to right) using random walk simulations (solid lines) and Gaussian approximation (dashed lines).¹



Temporal evolution of the concentration PDF for the linear reaction law ($\alpha=1$), spatially uncorrelated reaction rate constant $\kappa(x)$.²

Kinematic Wave (Saint-Venant) Equation

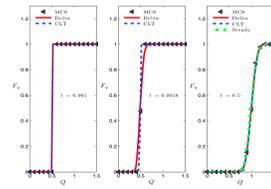
$$\frac{\partial c}{\partial t} + \frac{\partial q}{\partial x} = r(x, t), \quad q = \alpha c^{1/\beta}$$

Sources of Uncertainty:

- Surface slope and resistance $\alpha(x, t)$
- Measurement of turbulence β
- Sources $r(x, t)$
- Initial and boundary conditions

Effective CDF Equation:

$$\frac{\partial F_q}{\partial t} + \mathbf{v}_{\text{eff}} \cdot \nabla_{\mathbf{x}} F_q = \nabla_{\mathbf{x}} \cdot (\mathbf{D} \nabla_{\mathbf{x}} F_q)$$



Flow rate CDF computed with MCS, the white noise approximation (Delta), and the CLT-based approximation (CLT).³

Advective-Diffusive Transport

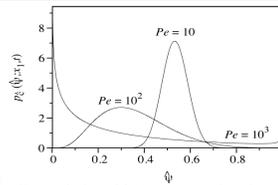
$$\frac{\partial c}{\partial t} = D \nabla^2 c - \nabla \cdot (\mathbf{u}c)$$

Map $p_c(\psi, \mathbf{x}, t)$ onto two observables:

- Center of mass of plume: $\mathbf{m}(t) \sim \int c(\mathbf{x}, t) \mathbf{x} dx_1 \cdots dx_d$
- Width of plume: $k_{ij}(t) \sim \int c(\mathbf{x}, t) x_i x_j dx_1 \cdots dx_d$

Particle trajectories $\mathbf{x}(t)$ follows a Langevin Equation:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{u}[\mathbf{x}(t), t] + \boldsymbol{\xi}(t), \quad \langle \xi_i(t) \xi_j(t') \rangle_\xi = 2D_{ij} \delta(t - t')$$



Concentration PDF for various Peclet numbers.⁴

Conclusions

- While standard techniques for uncertainty quantification typically yield only system state's mean and variance, the proposed approach leads to its full probabilistic description
- The shape of the PDF changes with time, varying between the known initial and steady-state distributions. This makes reliance on assumed PDFs problematic.
- PDF methods provide a computationally efficient means for uncertainty quantification.

References:

1. D. M. Tartakovsky, M. Dentz and P. C. Lichtner, "Probability density functions for advective-reactive transport in porous media with uncertain reaction rates", *Water Resour. Res.*, vol. 45, pp. W07414, 2009
2. D. M. Tartakovsky and S. Broyda, "PDF equations for advective-reactive transport in heterogeneous porous media with uncertain properties", *J. Contam. Hydrol.*, vol. 120-121, pp. 129-140, 2011
3. P. Wang, A. M. Tartakovsky and D. M. Tartakovsky, "Uncertainty quantification in kinematic wave models", *Submitted*.
4. M. Dentz and D. M. Tartakovsky, "Probability density functions for passive scalars dispersed in random velocity fields", *Geophys. Res. Lett.*, vol. 37, pp. L24406, 2010.

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