Response-excitation theory for stochastic ODEs and stochastic PDEs

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Overview

- Introduction to probability density function methods and their application to a simple stochastic advection problem.

- Hopf characteristic functional approach to nonlocal problems (e.g. diffusion problems) and derivation of differential constraints for the probability density function associated with the stochastic solution.

- Differential constraints for the probability density function of the wave equation and other PDEs subject to random boundary conditions, random initial conditions and random forcing terms.

- Classification of differential constraints: differential constraints depending on the specific stochastic field equation under consideration and intrinsic constraints depending only on the structure of the joint probability density function.

- Analytical verification of some differential constraints for random waves in a one-dimensional spatial domain.

- Brief discussion on the completeness of a set of differential constraints.

Functional integral representation of the probability density function associated with the solution to stochastic PDEs

In order to fix ideas, let us consider the nonlinear advection-diffusion problem

$$\begin{cases} \dfrac{\partial \psi}{\partial t} + \psi \dfrac{\partial \psi}{\partial x} = \nu \dfrac{\partial^2 \psi}{\partial x^2} \\ \psi(x, t_0; \omega) = \displaystyle\sum_{k=1}^{N} \eta_k(\omega) \Psi_k(x) \end{cases} \Rightarrow \quad \psi(x,t;\omega) = \psi(x,t;\eta_1(\omega), ..., \eta_N(\omega))$$

random input variables

The stochastic solution is a nonlinear functional of all the random input variables

The probability density function of the random variable $\psi(x,t;\omega)$, i.e. the stochastic solution at (x,t) , admits the following integral representation

$$\begin{aligned} p^{(a)}_{\psi(x,t)} &= \langle \delta\left(a - \psi(x,t;\eta_1, ..., \eta_N)\right) \rangle \\ &= \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \delta\left(a - \psi(x,t;z_1, ..., z_N)\right) \overbrace{w(z_1, ..., z_N)}^{\text{Joint PDF of } (\eta_1(\omega), ..., \eta_N(\omega))} dz_1 \cdots dz_N \end{aligned}$$

The integrals are formally from $-\infty$ to ∞ although the joint PDF may be compactly supported. If $N \to \infty$ we obtain the functional integral representation

$$p^{(a)}_{\psi(x,t)} = \int \underbrace{\mathcal{D}[z]}_{\text{Functional integral measure}} \underbrace{w[z]}_{\text{Probability density functional}} \delta\left(a - \psi(x,t;[z])\right)$$

Simple operations involving the probability density function

The Dirac delta function formalism allows us to perform various types of operations on the probability density function in a practical way. For instance,

Derivatives of one-point PDF	$\dfrac{\partial p^{(a)}_{\psi(x,t)}}{\partial t} = -\dfrac{\partial}{\partial a}\langle \delta(a-\psi)\psi_t\rangle \qquad \left(\psi_t \overset{\text{def}}{=} \dfrac{\partial \psi}{\partial t}(x,t;\omega)\right)$
Representation of the joint PDF of a field and its time derivative at different space-time locations	$p^{(a,b)}_{\psi(x,t)\psi_t(x',t')} = \langle \delta\left(a-\psi(x,t)\right)\delta\left(b-\psi_t(x',t')\right)\rangle$
Average of a continuous function of the field and its derivatives	$\langle \mathcal{H}(\psi,\psi_t)\delta\left(a-\psi\right)\delta\left(b-\psi_t\right)\rangle = \mathcal{H}(a,b)p^{(a,b)}_{\psi\psi_t}$
Time derivative of the Joint PDF of a field and its derivative at the same space-time location	$\dfrac{\partial}{\partial t}p^{(a,b)}_{\psi(x,t)\psi_t(x,t)} = -\dfrac{\partial}{\partial a}\langle \delta\left(a-\psi\right)\psi_t\delta\left(b-\psi_t\right)\rangle - \dfrac{\partial}{\partial b}\langle \delta\left(a-\psi\right)\psi_{tt}(x,t)\delta\left(b-\psi_t\right)\rangle$ $= -b\dfrac{\partial}{\partial a}p^{(a,b)}_{\psi(x,t)\psi_t(x,t)} - \dfrac{\partial}{\partial b}\langle \delta\left(a-\psi\right)\psi_{tt}(x,t)\delta\left(b-\psi_t\right)\rangle$

A. Khuri, ``Applications of Dirac's delta function in statistics'', *Int. J. Math. Edu. Sci. Tech.* **35**(2), 2004.

Nonlinear advection problem

Let us consider a prototype nonlinear advection problem with a random forcing term, random initial condition and periodic boundary conditions

Gaussian random variable

$$\begin{cases} \dfrac{\partial \psi}{\partial t} + \psi \dfrac{\partial \psi}{\partial x} = \dfrac{1}{2}\xi(\omega)\sin(x)\sin(20t)\,, \quad x \in [0, 2\pi]\,, \quad t \geq 0 \\ \psi(x, 0; \omega) = \dfrac{1}{2}\sin(x) + \eta(\omega) \\ \text{Periodic B.C.} \end{cases}$$

Gaussian random variable

The joint response-excitation probability density function for this system has the following integral representation

$$p^{(a,b)}_{\psi(x,t)\xi} = \langle \delta\left(a - \psi(x, t; [\xi, \eta])\right) \delta(b - \xi) \rangle$$

Average with respect to the joint measure of $\xi(\omega)$ and $\eta(\omega)$

A differentiation with respect to t and x gives

$$\frac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial t} = -\frac{\partial}{\partial a}\langle \delta(a - \psi)\psi_t \delta(b - \xi)\rangle$$

$$\frac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial x} = -\frac{\partial}{\partial a}\langle \delta(a - \psi)\psi_x \delta(b - \xi)\rangle \longrightarrow \langle \delta(a - \psi)\psi_x \delta(b - \xi)\rangle = -\int_{-\infty}^{a} \frac{\partial p^{(a',b)}_{\psi(x,t)\xi}}{\partial x} da'$$

Nonlinear advection problem in probability space

Also,

$$a\frac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial x} = -\frac{\partial}{\partial a}\langle\delta(a-\psi)\psi_x\psi\delta(b-\xi)\rangle + \langle\delta(a-\psi)\psi_x\delta(b-\xi)\rangle$$

i.e.

$$-\frac{\partial}{\partial a}\langle\delta(a-\psi)\left(\psi_t+\psi_x\psi\right)\delta(b-\xi)\rangle = \frac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial t} + a\frac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial x} + \int_{-\infty}^{a}\frac{\partial p^{(a',b)}_{\psi(x,t)\xi}}{\partial x}da'$$

Therefore, the joint response-excitation PDF associated with the solution to the nonlinear advection problem satisfies

$$\begin{cases} \dfrac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial t} + a\dfrac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial x} + \displaystyle\int_{-\infty}^{a}\frac{\partial p^{(a',b)}_{\psi(x,t)\xi}}{\partial x}da' = -\frac{1}{2}b\sin(x)\sin(20t)\frac{\partial p^{(a,b)}_{\psi(x,t)\xi}}{\partial a} \\ p^{(a,b)}_{\psi(x,t_0)\xi} = p_\eta(a,x)p_\xi(b) \\ \text{Periodic B.C.} \end{cases}$$

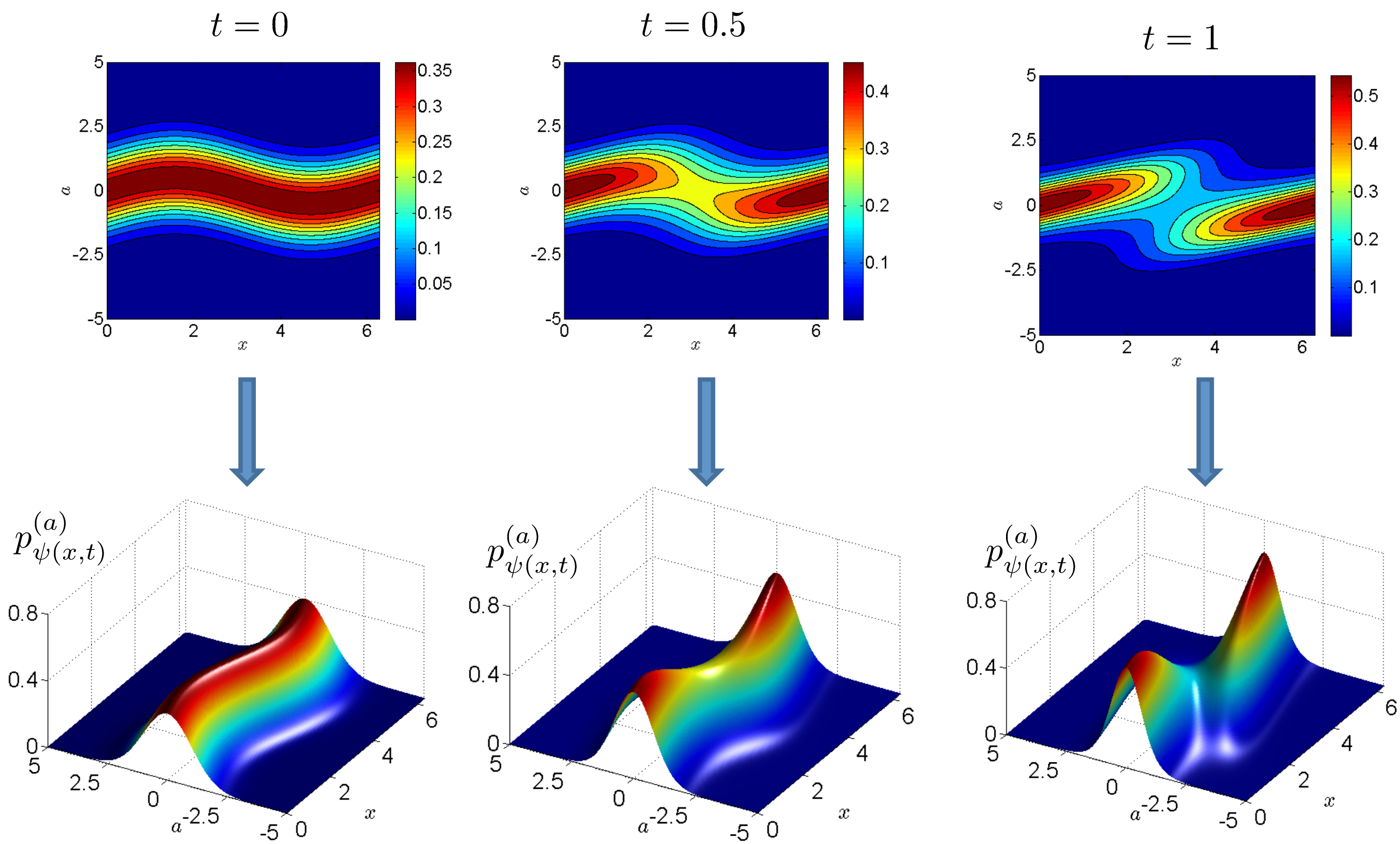
$$p_\xi(b) = \frac{1}{\sqrt{2\pi}}e^{-b^2/2}$$

$$p_\eta(a,x) = \frac{1}{\sqrt{2\pi}}e^{-(a-\sin(x)/2)^2/2}$$

Once the response-excitation PDF is available we can compute the response probability of the system and the statistical moments of the solution as

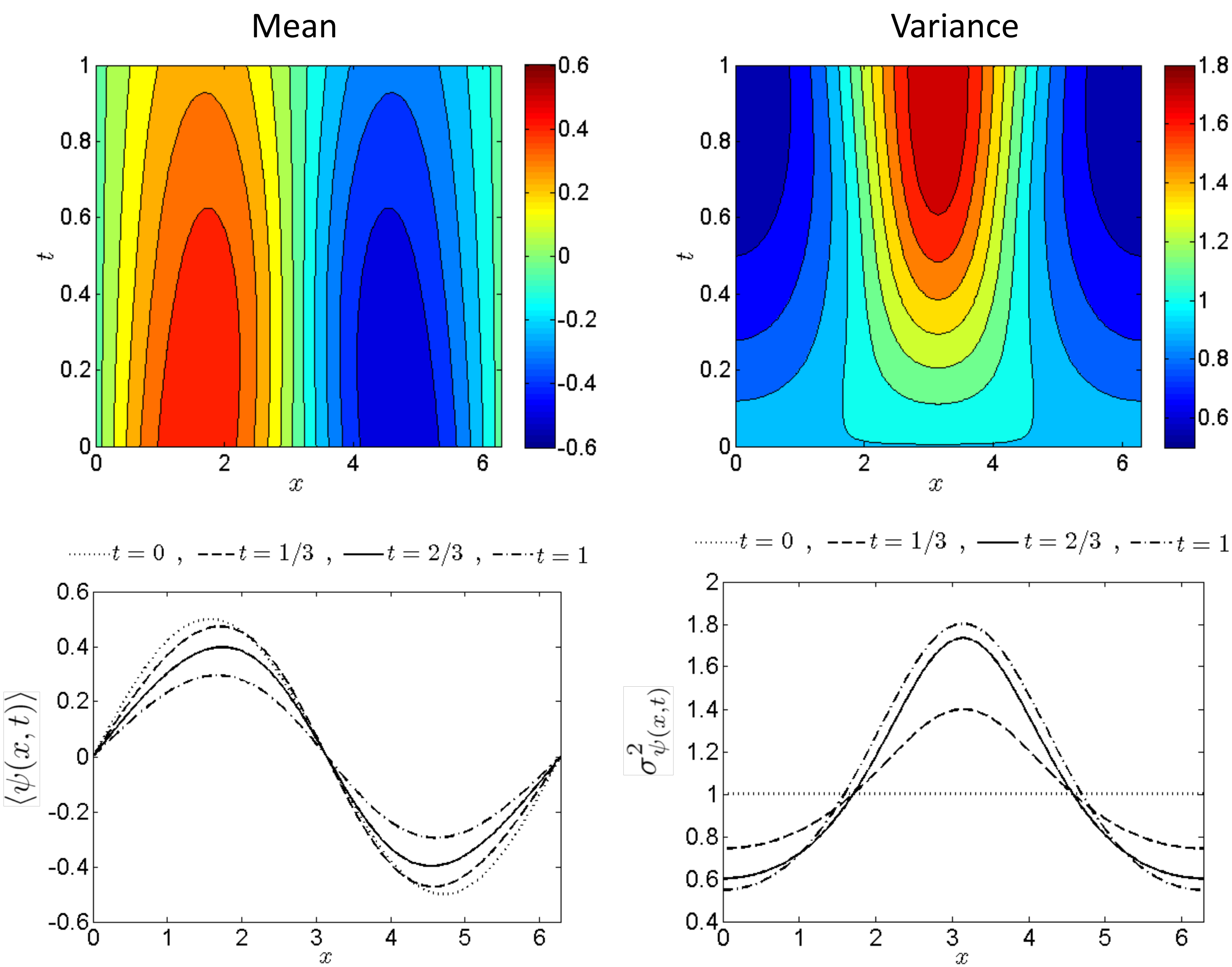
$$p^{(a)}_{\psi(x,t)} = \int_{-\infty}^{\infty}p^{(a,b)}_{\psi(x,t)\xi}db \qquad\qquad \langle\psi^n\rangle = \int_{-\infty}^{\infty}a^n p^{(a)}_{\psi(x,t)}da$$

Snapshots of the response probability density function



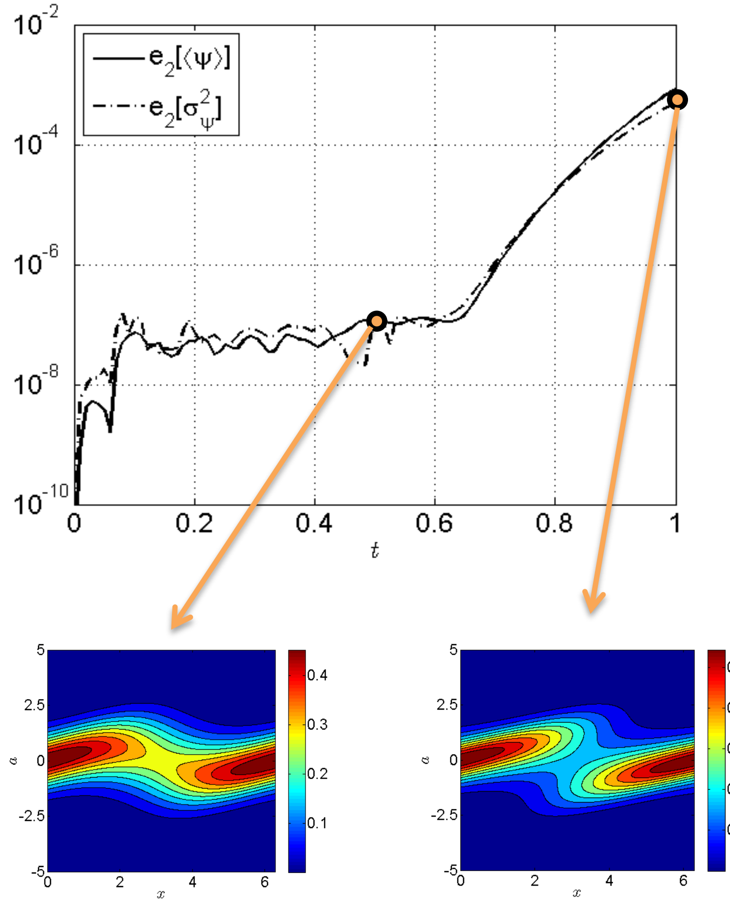
D. Venturi and G. E. Karniadakis, ``New evolution equations for the joint response-excitation probability density function of stochastic solutions to first-order nonlinear PDEs'', JCP, 2011 (Submitted)

Mean and variance of the stochastic solution

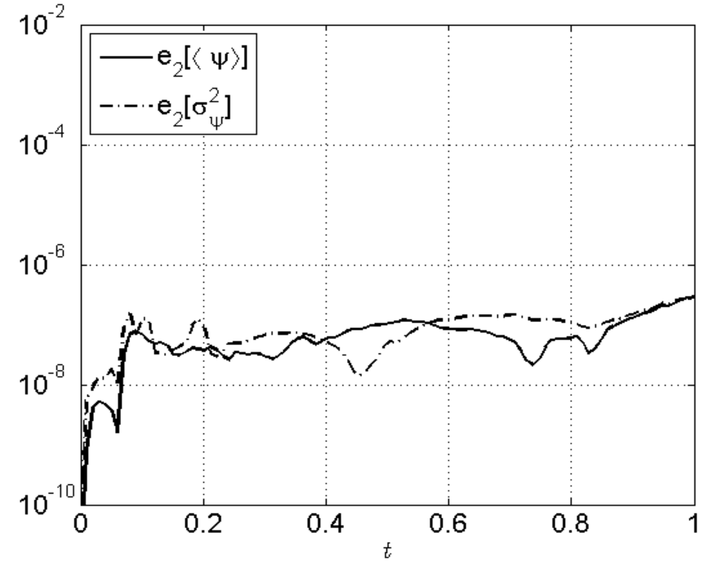


A Comparsion between ME-PCM and PDF method

PCM versus PDF



ME-PCM versus PDF



$$e_2[\langle\psi\rangle](t) = \frac{\|\langle\tilde{\psi}\rangle - \langle\psi\rangle\|_{L_2([0,2\pi])}}{\|\langle\psi\rangle\|_{L_2([0,2\pi])}}$$

$$e_2[\sigma_\psi^2](t) = \frac{\|\tilde{\sigma}_\psi^2 - \sigma_\psi^2\|_{L_2([0,2\pi])}}{\|\sigma_\psi^2\|_{L_2([0,2\pi])}}$$

The response PDF tends to split in two parts after time t=0.5. A global Gauss-Hermite probabilistic collocation method does not accurately capture the response statistics.

PCM: 50 Gauss-Hermite points (50x50 collocation points)
ME-PCM: 10 elements of order 10 (100x100 collocation points)

Some remarks

- In general, the computation of the statistical properties associated with the solution to a stochastic PDE subject to high-dimensional forcing, random boundary conditions or random initial conditions is a challenging problem.
- Standard stochastic approaches such as ME-PCM, sparse grid adaptive stochastic collocation or generalized spectral decompositions cannot generally overcome the curse of dimensionality.
- By using a PDF method, we have shown that first-order quasi-linear stochastic problems can be transformed into equivalent problems involving the joint response-excitation probability density function.

Is it possible to extend this method to arbitrary stochastic PDEs?

- Unfortunately, higher-order equations such as the advection-diffusion equation or the wave equation, do not admit a closed equation for the one-point probability density function associated with the stochastic solution.
- Therefore we are led to investigate the possibility to formulate an evolution problem for the probability density function in terms of a proper set of differential constraints.

A simple evolution equation yielding to nonlocal solutions

Let us consider a one-dimensional diffusion problem subject to random initial conditions of arbitrary dimensionality

$$\begin{cases} \dfrac{\partial \psi}{\partial t} = \alpha \dfrac{\partial^2 \psi}{\partial x^2}\,, \quad x \in \mathbb{R}\,, \quad t \geq 0 \\ \psi(x,0;\omega) = \psi_0(x;\omega) \end{cases}$$

The analytical solution can expressed in terms of Green functions as

$$\psi(x,t;\omega) = \int_{-\infty}^{\infty} \mathcal{G}(x,t|x')\psi_0(x';\omega)dx'$$

$$\mathcal{G}(x,t|x') = \frac{1}{(4\pi\alpha t)^{1/2}} \exp\left[-\frac{(x-x')^2}{4\alpha t}\right]$$

In this case computation of the statistical properties of the solution at a specific space-time location involves the full probability density functional of the initial condition ψ_0 .

In other words, when we try to advance in time the diffusion problem, we see that the PDF of the solution ψ at a specific space location depends on the joint probability of the solution at all spatial locations in the previous time step.

This suggests that the PDF of the solution of the diffusion problem do not satisfy a point-wise equation. It does satisfy, however, a functional differential equation.

Hopf characteristic functional approach

The full statistical information of the solution to the diffusion problem is encoded in the Hopf characteristic functional

$$F[\beta] = \langle Z[\beta] \rangle \qquad Z[\beta] = \exp\left[i \int_{-\infty}^{\infty} \int_{0}^{T} \overbrace{\psi(X,\tau;\omega)}^{\text{stochastic solution}} \underbrace{\beta(X,\tau)}_{\text{test field}} dX\, d\tau \right]$$

An evolution equation for $F[\beta]$ can be easily determined by using functional derivatives techniques, e.g.

$$\frac{\delta F[\beta]}{\delta \psi(x,t)} = i \langle \psi(x,t;\omega) Z[\beta] \rangle \quad \Rightarrow \quad \begin{cases} \dfrac{\partial}{\partial t} \dfrac{\delta F[\beta]}{\delta \psi(x,t)} = i \langle \psi_t(x,t;\omega) Z[\beta] \rangle \\[2ex] \dfrac{\partial^2}{\partial x^2} \dfrac{\delta F[\beta]}{\delta \psi(x,t)} = i \langle \psi_{xx}(x,t;\omega) Z[\beta] \rangle \end{cases}$$

Volterra functional derivative

$$\boxed{\frac{\partial}{\partial t} \frac{\delta F[\beta]}{\delta \psi(x,t)} = \alpha \frac{\partial^2}{\partial x^2} \frac{\delta F[\beta]}{\delta \psi(x,t)}}$$

This functional differential equation holds for every test field $\beta(x,t)$ and it cannot be reduced, in general, to a standard PDE for the one-point characteristic function or the PDF of the solution. Note that the structure of the functional differential equation is the same as the heat equation.

Differential constraints arising from the Hopf equation

We can equivalently consider the joint Hopf characteristic functional of ψ and ψ_x

$$F_2[\beta,\gamma] = \langle Z_2[\beta,\gamma] \rangle$$

$$Z_2[\beta,\gamma] = e^{i\int_{-\infty}^{\infty}\int_0^T \psi(X,\tau;\omega)\beta(X,\tau)dXd\tau + i\int_{-\infty}^{\infty}\int_0^T \psi_x(X,\tau;\omega)\gamma(X,\tau)dXd\tau}$$

and obtain

$$\frac{\partial}{\partial t}\frac{\delta F_2[\beta,\gamma]}{\delta\psi(x,t)} = \alpha\frac{\partial^2}{\partial x^2}\frac{\delta F_2[\beta,\gamma]}{\delta\psi(x,t)} \qquad\qquad \frac{\partial}{\partial x}\frac{\delta F_2[\beta,\gamma]}{\delta\psi(x,t)} = \frac{\delta F_2[\beta,\gamma]}{\delta\psi_x(x,t)}$$

These equations hold for arbitrary test fields $\beta(X,\tau)$ and $\gamma(X,\tau)$. In particular, they hold for

$$\beta^+(X,\tau) = a\delta(X-x)\delta(\tau-t) \qquad \text{and} \qquad \gamma^+(X,\tau) = b\delta(X-x)\delta(\tau-t) \qquad a,b\in\mathbb{R}$$

This yields the condition

$$\left\langle \left[\psi_t(x,t;\omega) - \alpha\psi_{xx}(x,t;\omega)\right] e^{ia\psi(x,t;\omega)+ib\psi_x(x,t;\omega)} \right\rangle = 0$$

which can be expressed in terms a differential constraint involving the joint characteristic function or, equivalently, the joint probability density function

$$p^{(a,b)}_{\psi(x,t)\psi_x(x',t')} = \langle \delta\left(a-\psi(x,t)\right)\delta\left(b-\psi_x(x',t')\right)\rangle$$

Differential constraints arising from the Hopf equation (2)

The result is

$$\boxed{\lim_{\substack{t'\to t\\ x'\to x}} \frac{\partial p^{(a,b)}_{\psi(t,x)\psi_x(x',t')}}{\partial t} = \alpha \lim_{\substack{t'\to t\\ x'\to x}} \frac{\partial^2 p^{(a,b)}_{\psi(t,x)\psi_x(x',t')}}{\partial x^2} - \alpha b^2 \frac{\partial^2 p^{(a,b)}_{\psi(t,x)\psi_x(x,t)}}{\partial a^2}}$$

Remarks

- This differential constraint has to be satisfied by the joint probability density function associated with every solution to the heat equation.
- It does not allow to determine uniquely the joint probability density of ψ and ψ_x.
- The joint probability density function of ψ and ψ_x satisfies also additional differential constraints which will be obtained hereafter for the prototype problem of a 1D wave equation.
- In order to determine these differential constraints we can use a more direct functional integral method which can be shown to be completely equivalent to the Hopf characteristic functional approach just illustrated.
- By evaluating the Hopf functional differential equation for test fields that are different from Dirac deltas we obtain other types of partial differential equations for the joint PDF.

Wave equation subject to random boundary conditions and random initial conditions

Let us consider the prototype problem of a one-dimensional wave equation subject to random boundary conditions or random initial conditions of arbitrary dimensionality

$$\frac{\partial^2 \psi}{\partial t^2} = U^2 \frac{\partial^2 \psi}{\partial x^2} \quad \Longrightarrow \quad \psi(x, t; \omega)$$

We define

$$\psi \stackrel{\text{def}}{=} \psi(x, t; \omega) \qquad \psi'_t \stackrel{\text{def}}{=} \frac{\partial \psi}{\partial t}(x', t'; \omega) \qquad \psi''_x \stackrel{\text{def}}{=} \frac{\partial \psi}{\partial x}(x'', t''; \omega)$$

and look for an evolution equation governing the joint probability density function

$$p^{(a,b,c)}_{\psi \psi'_t \psi''_x} = \langle \delta\left(a - \psi\right) \delta\left(b - \psi'_t\right) \delta\left(c - \psi''_x\right) \rangle \qquad \text{(9 variables)}$$

The average $\langle \cdot \rangle$ is defined as a functional integral with respect to the joint probability functional of the random initial condition and the random boundary conditions. In order obtain an equation for $p^{(a,b,c)}_{\psi \psi'_t \psi''_x}$ we differentiate it with respect to different independent variables and try to build up the wave equation within the average.

D. Venturi and G. E. Karniadakis, ``Differential constraints for the probability density function of stochastic solutions to the wave equation'', Int. J. for Uncertainty Quantification, 2011

Differential constraints depending on the wave equation (1)

By combining proper partial derivatives of $p^{(a,b,c)}_{\psi\psi'_t\psi''_x}$ we arrive at the following relation

$$\lim_{\substack{t',t''\to t\\ x',x''\to x}} \frac{\partial^2 p^{(a,b,c)}_{\psi\psi'_t\psi''_x}}{\partial t^2} = U^2 \lim_{\substack{t',t''\to t\\ x',x''\to x}} \frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x^2} + \left(b^2 - U^2 c^2\right) \frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a^2}$$

As before, this identity has to be satisfied by the joint PDF of every solution to the wave equation and it involves unusual partial differential operators which we shall call limit partial derivatives. For subsequent mathematical developments it is convenient to reserve a special symbol for these operators, i.e. we shall define

$$\frac{\mathfrak{d}^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d} t^2} \overset{\text{def}}{=} \lim_{\substack{t',t''\to t\\ x',x''\to x}} \frac{\partial^2 p^{(a,b,c)}_{\psi\psi'_t\psi''_x}}{\partial t^2} \qquad \frac{\mathfrak{d}^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d} x^2} \overset{\text{def}}{=} \lim_{\substack{t',t''\to t\\ x',x''\to x}} \frac{\partial^2 p^{(a,b,c)}_{\psi\psi'_t\psi''_x}}{\partial x^2}$$

This allows us to write the differential constraint in a PDE-like form

$$\boxed{\frac{\mathfrak{d}^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d} t^2} = U^2 \frac{\mathfrak{d}^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d} x^2} + \left(b^2 - U^2 c^2\right) \frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a^2}}$$

Differential constraints depending on the wave equation (2)

We can formulate another differential constraint depending on the wave equation. To this end, let us consider again the joint PDF

$$p^{(a,b,c)}_{\psi\psi'_t\psi''_x} = \left\langle \delta\left(a-\psi\right)\delta\left(b-\psi'_t\right)\delta\left(c-\psi''_x\right)\right\rangle$$

This time we differentiate it with respect to t' and x'' to obtain

$$\frac{\partial p^{(a,b,c)}_{\psi\psi'_t\psi''_x}}{\partial t'} = -\frac{\partial}{\partial b}\left\langle \delta\left(a-\psi\right)\psi'_{tt}\delta\left(b-\psi'_t\right)\delta\left(c-\psi''_x\right)\right\rangle$$

$$\frac{\partial p^{(a,b,c)}_{\psi\psi'_t\psi''_x}}{\partial x''} = -\frac{\partial}{\partial c}\left\langle \delta\left(a-\psi\right)\delta\left(b-\psi'_t\right)\delta\left(c-\psi''_x\right)\psi''_{xx}\right\rangle$$

Combining these two results and taking the wave equation into account yields the differential constraint

$$\boxed{\frac{\partial}{\partial c}\frac{\mathfrak{d} p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d} t'} = U^2\frac{\partial}{\partial b}\frac{\mathfrak{d} p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d} x''}}$$

Thanks to a set of additional differential constraints arising form the structure of the probability density function it can be shown that this constraint is equivalent to the one involving second order limit partial derivatives (previous slide).

An equation for the response probability density

If we integrate the differential constraint

$$\frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial t^2} = U^2 \frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x^2} + \left(b^2 - U^2 c^2\right) \frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a^2}$$

with respect to b and c we obtain the evolution equation for the response probability density, i.e., the probability density of the random wave ψ

$$p^{(a)}_{\psi(x,t)} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p^{(a,b,c)}_{\psi\psi'_t\psi''_x}\, dbdc = \langle \delta(a-\psi)\rangle$$

$$\frac{\partial^2 p^{(a)}_{\psi(x,t)}}{\partial t^2} = U^2 \frac{\partial^2 p^{(a)}_{\psi(x,t)}}{\partial x^2} + \frac{\partial^2}{\partial a^2}\langle \delta(a-\psi)\psi_t^2\rangle - U^2 \frac{\partial^2}{\partial a^2}\langle \delta(a-\psi)\psi_x^2\rangle$$

This equation is not closed. Thus, in order to compute $p^{(a)}_{\psi}$ we need a closure approximation of the two averages above. This approximation can be constructed, e.g., by expanding the two averages in a functional power series.

- G. N. Bochkov, A. A. Dubkov and A. N. Malakhov, ``Structure of the correlation dependence of nonlinear stochastic functionals'', *Radiophysics and Quantum Electronics*, **20**(3), pp. 276-280, 1977.
- H. Chen, S. Chen and R. H. Kraichnan, ``Probability distribution of a stochastically advected scalar field'', *Phys. Rev. Lett.*, **63**, pp. 2657-2660, 1989.
- 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

Intrinsic constraints depending on the structure of the joint PDF

The fields appearing in the joint density are, in general, related to each other. For instance,

$$p^{(a,b,c)}_{\psi\psi'_t\psi''_x} = \langle \delta\left(c - \psi''_x\right) \delta\left(b - \psi'_t\right) \delta\left(a - \psi\right) \rangle$$

$$\psi_x(x,t;\omega) = \lim_{x'\to x} \frac{\psi(x',t;\omega) - \psi(x,t;\omega)}{x' - x}$$

$$\boxed{\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x} = -c\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a}}$$

(Intrinsic constraints)

$$p^{(a,b,c)}_{\psi\psi'_t\psi''_x} = \langle \delta\left(c - \psi''_x\right) \delta\left(b - \psi'_t\right) \delta\left(a - \psi\right) \rangle$$

$$\psi_t(x,t;\omega) = \lim_{t'\to t} \frac{\psi(x,t';\omega) - \psi(x,t;\omega)}{t' - t}$$

$$\boxed{\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial t} = -b\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a}}$$

Similarly it can be shown that existence of ψ_{xx} and ψ_{tt} implies that

$$\int_{-\infty}^{a} \frac{\partial^2 p^{(a',b,c)}_{\psi\psi_t\psi_x}}{\partial x^2} da' = c^2 \frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a} + \int_{-\infty}^{c} \frac{\partial p^{(a,b,c')}_{\psi\psi_t\psi_x}}{\partial x''} dc'$$

$$\int_{-\infty}^{a} \frac{\partial^2 p^{(a',b,c)}_{\psi\psi_t\psi_x}}{\partial t^2} da' = b^2 \frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a} + \int_{-\infty}^{b} \frac{\partial p^{(a,b',c)}_{\psi\psi_t\psi_x}}{\partial t'} db'$$

If ψ is analytic in t and x then an infinite number of intrinsic differential constraints (depending only on the structure of the joint PDF) can be formulated.

A summary of differential constraints involving the joint PDF

We summarize here some differential constraints we have obtained so far

$$\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x} = -c\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a}$$

$$\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial t} = -b\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a}$$

$$\int_{-\infty}^{b} \frac{\partial p^{(a,b',c)}_{\psi\psi_t\psi_x}}{\partial x'} db' = \int_{-\infty}^{c} \frac{\partial p^{(a,b,c')}_{\psi\psi_t\psi_x}}{\partial t''} dc'$$

$$\int_{-\infty}^{a} \frac{\partial^2 p^{(a',b,c)}_{\psi\psi_t\psi_x}}{\partial x^2} da' = c^2\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a} + \int_{-\infty}^{c} \frac{\partial p^{(a,b,c')}_{\psi\psi_t\psi_x}}{\partial x''} dc'$$

$$\int_{-\infty}^{a} \frac{\partial^2 p^{(a',b,c)}_{\psi\psi_t\psi_x}}{\partial t^2} da' = b^2\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a} + \int_{-\infty}^{b} \frac{\partial p^{(a,b',c)}_{\psi\psi_t\psi_x}}{\partial t'} db'$$

Constraints depending only on the structure of the joint probability density function

$$\frac{\partial}{\partial c}\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial t'} = U^2\frac{\partial}{\partial b}\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x''}$$

$$\frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial t^2} = U^2\frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x^2} + \left(b^2 - U^2c^2\right)\frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a^2}$$

Constraints depending on the wave equation

Numerical issues in the simulation of a boundary value problem for the joint response-excitation PDF

- The support of the joint response excitation probability density may be a compact set.

- Deterministic boundary and initial conditions are associated with Dirac delta functions in probability space. The numerical simulation of an equation involving Dirac delta function is a challenging problem.

- The boundary conditions and the initial conditions for the joint response-excitation density are nonlocal. This means that if we need to set, e.g. a Dirichlet boundary condition in physical space, then the corresponding condition in probability space is set for

$$p^{(a)}_{\psi(x,t)} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p^{(a,b,c)}_{\psi\psi'_t\psi''_x}\, db\, dc$$

- The joint response excitation density could be a discontinuous function.

An analytical example – waves in 1D infinite domains

Consider the boundary value problem

$$\begin{cases} \dfrac{\partial^2 \psi}{\partial t^2} = U^2 \dfrac{\partial^2 \psi}{\partial x^2}\,, \quad -\infty < x < \infty\,, \quad t \geq t_0 \\ \psi(x, t_0; \omega) = \sum_{k=1}^{3} \underbrace{\xi_k(\omega)}_{\text{Jointly Gaussian RVs}} \underbrace{h_k(x)}_{\text{e.g.}} \\ \psi_t(x, t_0; \omega) = 0 \end{cases}$$

Jointly Gaussian RVs

e.g.

$$\begin{cases} h_1(x) = \dfrac{3}{2} e^{-x^2/2} \\ h_2(x) = \sin(x^2) \\ h_3(x) = \cos(3x) \end{cases}$$

The solution is the well-known d'Alambert wave

$$\psi(x, t; \omega) = \frac{1}{2} \sum_{k=1}^{3} \xi_k(\omega) \left[h_k\left(x + Ut\right) + h_k\left(x - Ut\right) \right]$$

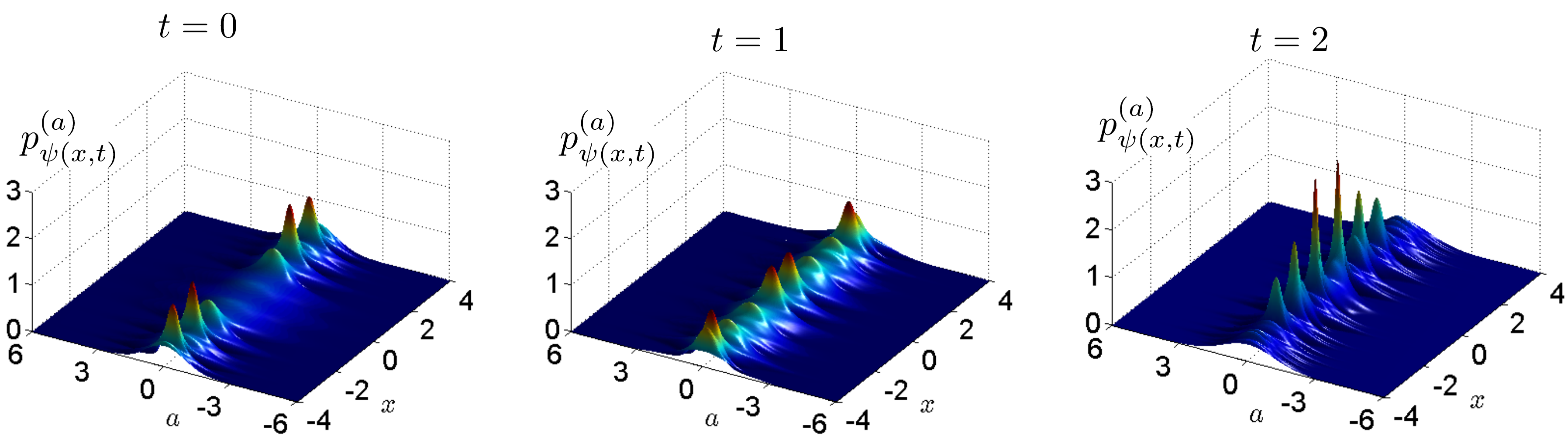
The joint probability of ψ , ψ'_t and ψ''_x can be obtained by using the mapping approach

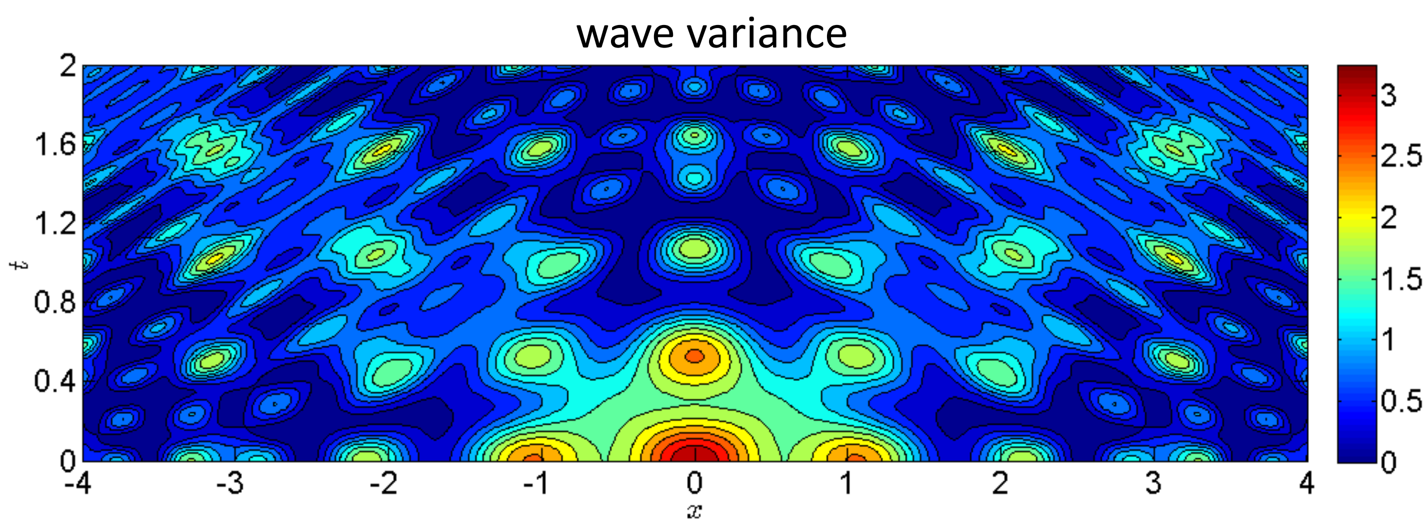
$$\begin{tikzcd} \{\xi_1, \xi_2, \xi_3\} \arrow[r] \arrow[d, "\text{3D Linear transformation}"'] & p^{(a,b,c)}_{\xi_1 \xi_2 \xi_3} \arrow[d, "\text{Jacobian}"] \\ \{\psi, \psi'_t, \psi''_x\} \arrow[r] & p^{(a,b,c)}_{\psi \psi'_t \psi''_x} = \dfrac{1}{|J|} p^{(\hat{\alpha}_1, \hat{\alpha}_2, \hat{\alpha}_3)}_{\xi_1 \xi_2 \xi_3} \end{tikzcd}$$

$$\hat{\alpha}_i(x, t, x', t', x'', t''; a, b, c)$$

Snapshots of the response probability density function

$$p^{(a)}_{\psi(x,t)} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} p^{(a,b,c)}_{\psi\psi'_t\psi''_x} dbdc$$





An analytical verification of a simple differential constraint

Let us show that the joint PDF of the random wave satisfies

$$\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x} = -c\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a}$$

$$\hat{\alpha}_i(x,t,x',t',x'',t'';a,b,c)$$

To this end we recall that $\quad p^{(a,b,c)}_{\psi\psi'_t\psi''_x} = \frac{1}{|J|}p^{(\hat{\alpha}_1,\hat{\alpha}_2,\hat{\alpha}_3)}_{\xi_1\xi_2\xi_3}$

$$J(x,t,x',t',x'',t'')$$

We have

$$\begin{aligned}
\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial x} &= -\frac{1}{J\,|J|}\overbrace{\frac{\partial J}{\partial x}}^{=0}p^{(\hat{\alpha}_1,\hat{\alpha}_2,\hat{\alpha}_3)}_{\xi_1\xi_2\xi_3} + \frac{1}{|J|}\frac{\partial p^{(\hat{\alpha}_1,\hat{\alpha}_2,\hat{\alpha}_3)}_{\xi_1\xi_2\xi_3}}{\partial\widehat{\alpha}_i}\frac{\partial\widehat{\alpha}_i}{\partial x} \\
&= \frac{1}{|J|}\frac{\partial p^{(\hat{\alpha}_1,\hat{\alpha}_2,\hat{\alpha}_3)}_{\xi_1\xi_2\xi_3}}{\partial\widehat{\alpha}_i}\frac{\partial\widehat{\alpha}_i}{\partial x} \\
&= -\frac{c}{|J|}\frac{\partial p^{(\hat{\alpha}_1,\hat{\alpha}_2,\hat{\alpha}_3)}_{\xi_1\xi_2\xi_3}}{\partial\widehat{\alpha}_i}\frac{\partial\widehat{\alpha}_i}{\partial a} \\
&= -c\frac{\partial p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a}
\end{aligned}$$

$$\frac{\partial\widehat{\alpha}_i}{\partial x} = -c\frac{\partial\widehat{\alpha}_i}{\partial a}$$

The proof of this relation is rather complex and it is not presented here

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- D. Venturi and G. E. Karniadakis, ``Differential constraints for the probability density function of stochastic solutions to the wave equation'', Int. J. for Uncertainty Quantification, 2011

Is the set of differential constraints complete?

The differential constraints we have obtained are identically satisfied by the joint probability density function associated with the solution to the stochastic wave equation. At this point we pose the fundamental question:

Is it possible to compute the probability density function of the wave as the solution to a suitable set of differential constraints? How many of them do we need in order to have a complete system?

- It can be shown that a boundary value problem involving only one constraint is ill-posed, i.e., it admits an infinite number of solutions.

$$\frac{\mathfrak{d}^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d}t^2} = U^2 \frac{\mathfrak{d}^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\mathfrak{d}x^2} + \left(b^2 - U^2 c^2\right) \frac{\partial^2 p^{(a,b,c)}_{\psi\psi_t\psi_x}}{\partial a^2}$$

- In the next slide we show that the set of constraints involving limit partial derivatives of first-order with respect to all variables is complete for first-order nonlinear stochastic PDEs .

- It is still an open question if the set of first-order differential constraints is complete for higher-order nonlinear stochastic PDEs.

A complete set of first-order differential constraints

$$\frac{\partial\psi}{\partial t}+\left(\frac{\partial\psi}{\partial x}\right)^2=0 \quad \Longrightarrow \quad p^{(a,b)}_{\psi\psi'_x}=\langle\delta\left(a-\psi\right)\delta\left(b-\psi'_x\right)\rangle$$

The full set of first-order differential constraints is

$$\begin{cases} \dfrac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}t}=b^2\dfrac{\partial p^{(a,b)}_{\psi\psi_x}}{\partial a} \\ \dfrac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}t'}=\dfrac{\partial}{\partial b}\left(2b\langle\delta(a-\psi)\delta(b-\psi_x)\psi_{xx}\rangle\right) \\ \dfrac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}x}=-b\dfrac{\partial p^{(a,b)}_{\psi\psi_x}}{\partial a} \\ \dfrac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}x'}=-\dfrac{\partial}{\partial b}\langle\delta(a-\psi)\delta(b-\psi_x)\psi_{xx}\rangle \end{cases}$$

$$\frac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}t'}=-\frac{\partial}{\partial b}\left(2b\int_{-\infty}^{b}\frac{\mathfrak{d}p^{(a,b')}_{\psi\psi_x}}{\mathfrak{d}x'}db'\right)$$

Taking into account the relations

$$\frac{\partial p^{(a,b)}_{\psi\psi_x}}{\partial x}=\frac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}x}+\frac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}x'} \qquad \frac{\partial p^{(a,b)}_{\psi\psi_x}}{\partial t}=\frac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}t}+\frac{\mathfrak{d}p^{(a,b)}_{\psi\psi_x}}{\mathfrak{d}t'}$$

we obtain

$$\boxed{\frac{\partial p^{(a,b)}_{\psi\psi_x}}{\partial t}=b^2\frac{\partial p^{(a,b)}_{\psi\psi_x}}{\partial a}-\frac{\partial}{\partial b}\left[2b\left(\int_{-\infty}^{b}\frac{\partial p^{(a,b')}_{\psi\psi_x}}{\partial x}db'+\int_{-\infty}^{b}b'\frac{\partial p^{(a,b')}_{\psi\psi_x}}{\partial a}db'\right)\right]}$$

This is the closed and exact evolution equation for the joint PDF of the system

Conclusions

- **First-order** nonlinear and quasi-linear scalar stochastic PDEs always admit a reformulation in terms of a linear evolution equation involving the one-point probability density function. Such equation can be solved efficiently using methods for high-dimensional problems such as sparse grid or proper generalized decomposition. Furthermore, if randomness come only from boundary or initial conditions then a PDF method can overcome the curse of dimensionality problem.

- However, **higher-order** stochastic PDEs such as the wave equation do not admit, in general, a corresponding closed evolution equation for the PDF associated with the solution at a specific space-time location. In these cases one can resort to closure approximations or even try to solve numerically the Hopf functional differential equation for the probability density functional of the solution.

- In this talk we have developed a new methodology that allows us to obtain a set of differential constraints satisfied by the PDF associated with the solution to a stochastic PDE. The set of these differential constraints was shown to be complete for first-order stochastic PDEs, i.e. it allows to compute uniquely the PDF of the system.

- It is still an open question if there exist a set of differential constraints, e.g. the one involving first-order limit partial derivatives with respect to all variables, that allows to determine uniquely the probability density function of the solution to higher-order nonlinear SPDEs.