Quantifying Uncertainty

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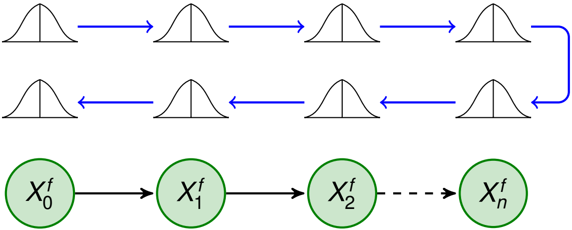
Organization

- Project: Two MCMC applications
- Lecture
- Next Meet: Project Updates

Content

- Model Reduction Wrap up
- Response Surface Modeling
- Polynomial Chaos

Uncertainty Propagation in Causal Systems



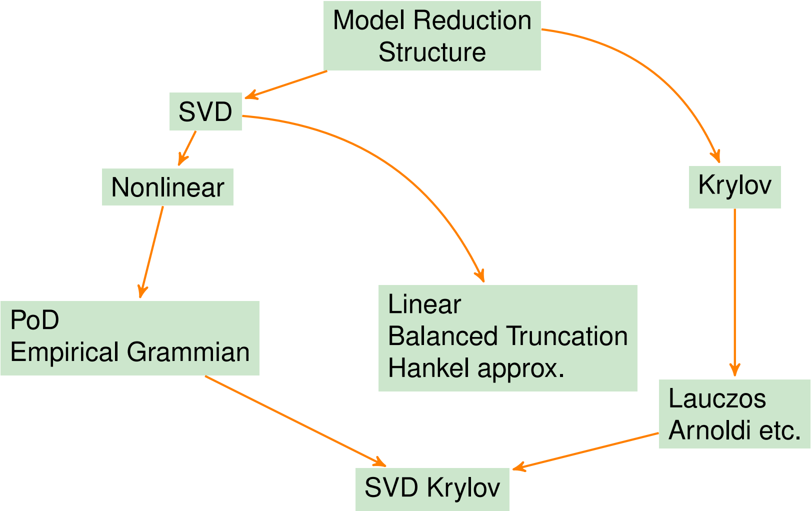
$$M \equiv M(X_t; \alpha_t)$$

$$X_{t+1} = M(X_t; \alpha_t) + \omega_t$$

$M \rightarrow$ Physical Model

$\rightarrow$ $(Estimated) Statistical Model$

Model Reduction



$$\frac{\partial\theta}{\partial t}(x,t) = D\theta(x,t) \rightarrow \textit{System}$$

$$R(\theta) = \frac{\partial\theta}{\partial t} - D\theta \rightarrow \textit{Residual}$$

$$\theta = u\eta(t) \rightarrow \text{KLT (POD or Krylov)}$$

$$u^T R = 0 \rightarrow \text{Galerkin Projection}$$

$$\frac{\partial\eta}{\partial t} = u^T D u\eta \rightarrow \textit{ROM}$$

K-L Theorem

Recall

$$\underline{Y}(t) = \underline{\underline{u}}\,\underline{\underline{\lambda}}\,\underline{\eta}[t]$$

or

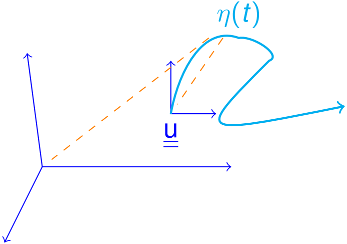
$$y(x,t) = \sum_{i=1}^{\infty(N)} u(i)\lambda(i)\eta(i,t)$$

K-L Contd.

We understand that

$\underline{u} \rightarrow$ over space

$\eta \rightarrow$ over time



AND

$$C(x_1, x_2) = \sum_{i=1}^{\infty (N)} \lambda_i^2 u_i(x_1) u_i(x_2)$$

$$\boxed{\underline{\underline{C}} \equiv \underline{\underline{u}}\,\underline{\underline{\lambda}}^2 \underline{\underline{u}}^T}$$

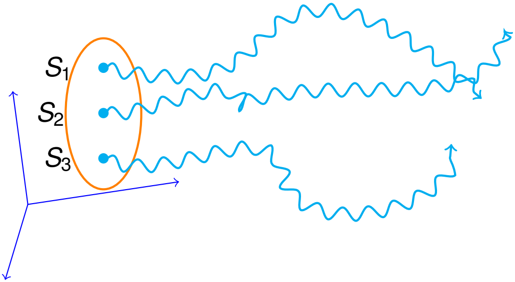
$$uu^T = u^T u = I$$

&

$$\underline{\underline{C}}\,\underline{\underline{u}} = \underline{\underline{\lambda}}\,\underline{\underline{u}}$$

Extension

What about Stochastic Process?



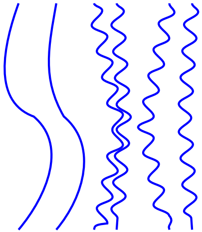
$$\underline{Y}[s,t] \equiv y(x,\underline{t},\underline{S})$$

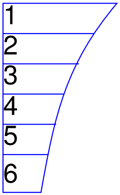
K-L works fine:

$$\underline{Y}[t,s] = \underline{\underline{u}}\,\underline{\underline{\lambda}}\,\underline{\eta}[t,s]$$
$$= \underline{\underline{u}}\,\underline{\underline{\chi}}[t,s]$$

What if

$$\underline{Y} = \underline{\underline{u}}\,\underline{w}$$





Or

$$y(x) = \sum_{i=1}^{\infty} w_i u_i(x)$$

Now let

$$y(x) \approx \hat{y}(x) = \underbrace{\sum_{i=1}^{N} w_i u_i(x)}_{approximated}$$

Residual

$$\Rightarrow R(x) \equiv y - \hat{y} = y(x) - \sum_{i=1}^{N} w_i u_i(x)$$

Galerkin Projection

$$\int R(x)u_j(x)dx = 0$$

Errors are orthogonal to basis

$$\Rightarrow \int_x \left[y(x) - \sum_i w_i \, u_i(x) \right] u_j(x)dx = 0$$

Galerkin Projection Contd.

Orthoganality condition in u

$$\int_x u_i(x)\, u_j(x) = \delta_{ij}$$

So, we get:

$$\int_x [y(x)\, u_j(x)]\, dx - w_j = 0$$

Contd.

Or

$$w_j - \int_x u_j(x)\, y(x) dx$$

$$\boxed{\underline{w} = \underline{\underline{u}}^T \underline{y}}$$

What is u?

How to evaluate the integral?

Gaussian Quadrature

$$w_j = \int_x u_j(x)y(x)dx = \sum_i u_j(x_i)y(x_i)v_j$$

or

$$\int_x R(x)u_j(x) = \sum_{i=1}^{c} u_j(x_i)R(x_i)v_j = 0 \quad \forall j$$

x_i-Collocation points

Quadrature leads us out

let $V_i \equiv V(x_i)$

$$\sum_{i=1}^{c} u_j(x_i) \left[y(x_i) - \sum_{k=1}^{N} w_k \, u_k(x_i) \right] V(x_i)$$

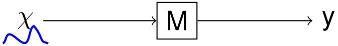
$$= \sum_{i=1}^{c} \left[u_j(x_i) y(x_i) V(x_i) - \underbrace{\sum_{k=1}^{N} w_k u_k(x_i) u_j(x_i) V(x_i)}_{\text{consider this term}} \right]$$

$$\sum_{k=1}^{N} w_k \sum_{i=1}^{c} u_k(x_i) u_j(x_i) V(x_i) = \begin{cases} 0 & k \neq j \\ w_j & k = j \end{cases}$$

$$\begin{aligned} \sum_{i=1}^{c} u_k(x_i) u_j(x_i) V(x_i) &= 0 \quad k \neq j \\ &= 1 \quad k = j \end{aligned}$$

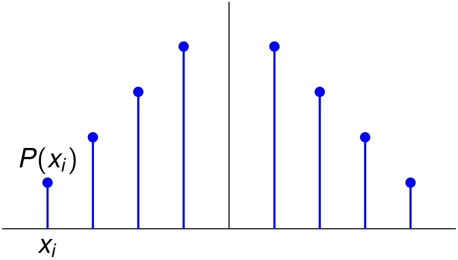
$$\left.\begin{aligned} u &= Orthogonal \\ x_i &= Collocation \\ V(x_i) &= Weights! \end{aligned}\right] \text{How to determine?}$$

Let us assume $\chi = \chi(\xi)$, a r.v.



a random input

So, we may let $V(x_i) = P(x_i)$



$u_j \equiv$ Orthogonal Polynomials

- If $x(\xi) \sim N(\cdot)$, Then $u \Rightarrow$ Hermite Polynomials
- And $\{x_i\} \Rightarrow$ Roots of (N+1) polynomial
- Can we do better?

“STOCHASTIC COLLOCATION”

R.v. x(ξ)	Wiener-Asky PC	Support
Gaussian	Hermite	$(-\infty, \infty)$
Gamma	Laguerre	$[0, \infty]$
Beta	Jacobi	[a,b]
Uniform	Legendre	[a,b]
Poisson	Charlier	{0,1,2,. . . }
Binomial	Krawtchouk	{0,1,2,. . . N}
Hypergeometric	Hahn	{0,1,2,. . . ,N}

- How to get coefficients?
- How to get good collocation points?

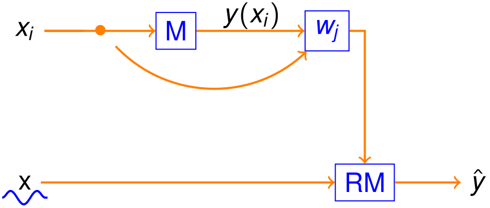
SCM or PCM

$$y(z,t,\xi) = \sum_{i=0}^{N} w(z,t,\{\xi_i\})u(\{\xi_i\})$$

This general form is the same as what we have discussed.

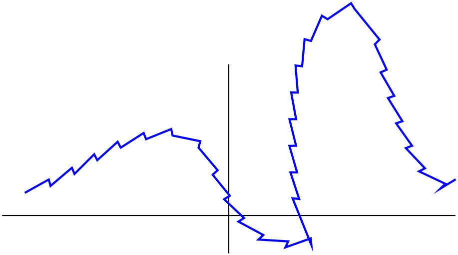
Coefficients

$$w_j = \sum_i u_j(x_i) y(x_i) v(x - i)$$



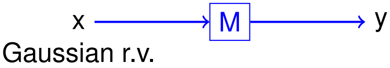
$$\hat{y}(x) = \sum_{i=1}^{N} u_i(x) w_i \quad \Rightarrow \textit{Fast}$$

Is it too good to be true?



How smooth must y be?

Other Methodology



$$y = w_0 + \sum_{i=1}^{N} w_i \, u_i(x)$$

$$U_i(x) = \underbrace{(-1)^i e^{\frac{1}{2}x^2} \frac{\partial}{\partial x^i} e^{-\frac{1}{2}x^2}}_{\text{Hermites Polynomials}}$$

$$
\begin{aligned}
y^{(1)} &= w_0 + xw_1 \\
y^{(2)} &= w_0 + xw_1 + w_2(x^2 - 1) \\
y^{(3)} &= y^{(2)} + (x^3 - 3x)w_3 \\
y^{(4)} &= y^{(3)} + \vdots
\end{aligned}
$$

Can iteratively refine!

$$\begin{bmatrix} y_1^{(3)} \\ y_2^{(3)} \\ y_3^{(3)} \\ y_4^{(3)} \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 - 1 & x_1^3 - 3x_1 \\ 1 & x_2 & x_2^2 - 1 & x_2^3 - 3x_2 \\ 1 & x_3 & x_3^2 - 1 & x_3^3 - 3x_3 \\ 1 & x_4 & x_4^2 - 1 & x_4^3 - 3x_4 \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

Solve

$$\underline{Y} = \underline{\underline{M}}\,\underline{w}$$

Can be iterative

Collocation vs Regression

Not Intrusive: Compare with model reduction

Too many points: If there are d variables (dimensions) and order p, there are $(p+1)^d$ points (grows quickly!)

Also: Collocation in the Gauss-Quadrature can not be reused u_k & u_{k+1} don't share roots!

Are collocation points highly probable?

In multiple dimensions (two)

$$
\begin{aligned}
y^{(1)} &= a_0 + a_{1_1} x_1 + a_{1_2} x_2 \\
y^{(2)} &= y^{(1)} + a_{2_1}(x_1^2 - 1) + a_{2_2}(x_2^2 - 1) \\
&\quad + a_{2_3} x_1 x_2 \\
y^{(3)} &= y^{(2)} + \dots
\end{aligned}
$$

What's going on?

Recall

$$\begin{aligned} w_j &= \int_x u_j(x)y(x)dx \\ &= \sum_i u_j(x_i)y(x_i)v(x_i) \\ &= \sum_i y(x_i)H_j(x_i)G(x_i) \end{aligned}$$

$H_j(x_i)$ -Hermite Polynomial

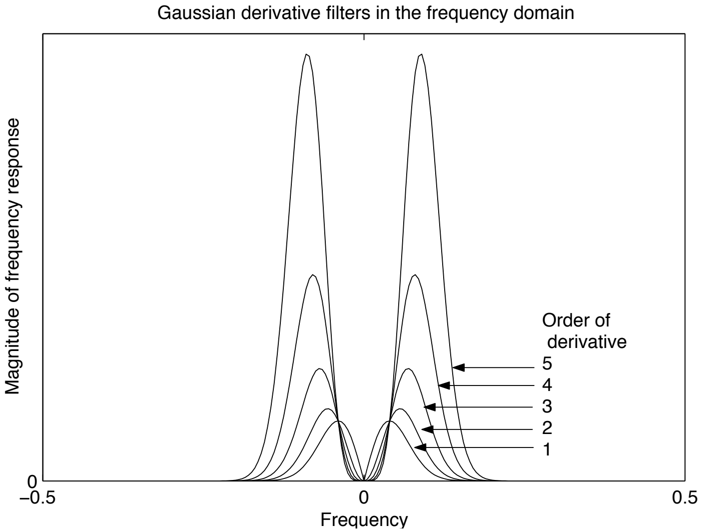
$G(x_i) \rightarrow e^{\frac{-x_i^2}{2}}$

Contd.

$$
\begin{aligned}
w_j &= \sum_i y(x_i) \frac{\partial^j}{\partial x^j} G(x_i) \\
&= \underbrace{Y \circledast \frac{\partial^j G}{\partial x^j}}_{\substack{\text{convolution by a} \\ \text{Gaussian derivative!}}} \\
&= \frac{\partial^j Y}{\partial x^j} \circledast G \rightarrow \text{smoothed derivatives}
\end{aligned}
$$

So, if you had a surface Y, response surface, then the “weights” are the filtered responses of Y with Gaussian derivative filters.

FROM MY THESIS ⇓


Gaussian derivative filters in the frequency domain
Magnitude of frequency response
Frequency
0
–0.5
0
0.5
Order of
derivative
5
4
3
2
1

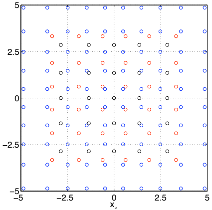
Back to multiple dimensions

in “n” dimensions:

$$Y^{(2)} = w_0 + \sum_{i=1}^{n} w_{ii}(x_i^2 - 1) + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} x_i x_j$$

Back to Collocation

Gauss-quadrature is not nested



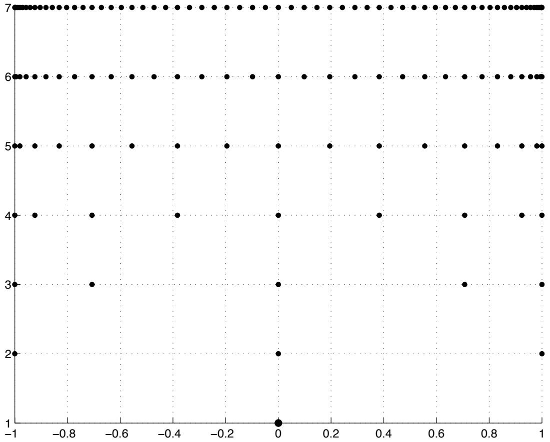
Non Gaussian rvs.

1. Choose from Askey scheme
2. Transform rvs some how

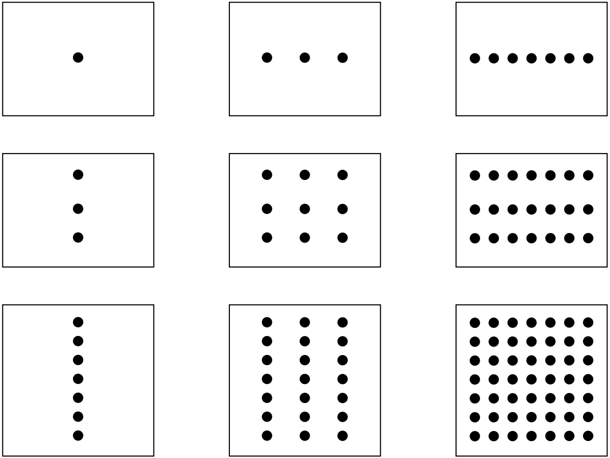
e.g: By decorrelation in case of correlated r.v.s

$$\widetilde{X} = usv'$$
$$\tilde{x} = \sqrt{s}u^T\widetilde{X}$$

Clenshaw-Curtis



Smolyak

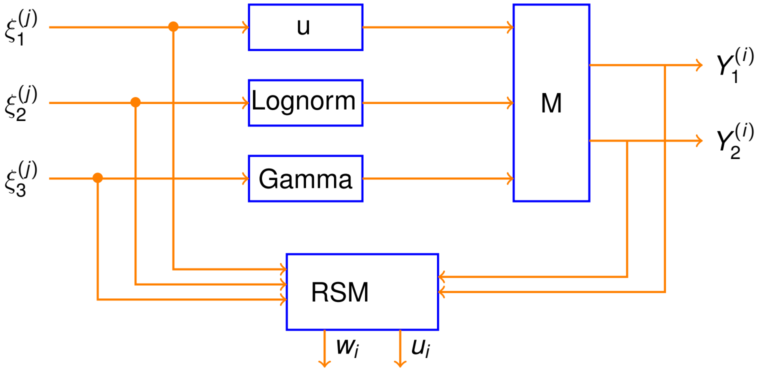


Other Transformations

$\xi \sim N(0,1)$

$U(a,b)$	$a+(b-a)\left[\frac{1}{2}+\frac{1}{2}erf(\frac{\xi}{\sqrt(2)})\right]$
$Lognormal(\mu,\sigma)$	$exp(\mu+\sigma\xi)$
$Gamma(a,b)$	$ab\left(\xi\int\frac{1}{9a}+1-\frac{1}{9a}\right)$
$Exponential(\lambda)$	$-\frac{1}{\lambda}\log\left(\frac{1}{2}+\frac{1}{2}erf\left(\frac{\xi}{\sqrt(2)}\right)\right)$
$Weibull(a)$	$\xi^{1/a}$
Extreme Value	$-\log(\xi)$

Example



Convergence

$||\hat{y}_n - y|| \rightarrow$Convergence in L_2
Not in any norm

Summary

- Quick & Easy UQ
- Non-Intrusive
- Time?
- Basis optimality (e.g. wavelets)

- Smooth Response Surface
- Not Significant nonlinearity
- Bifurcations in rv
- Grids!

Polynomial Chaos Expansion

SCM very different from PCE/gPC

$$Y(x,t,\xi) = \sum_{i=0}^{\infty(N)} \underbrace{y_i(x,t)}_{Deterministic} \cdot \underbrace{\psi_i(\xi)}_{Stochastic}$$

So PCE by construction/an assumed solution. SCM/PCM from quadrature!

Contd.

- $\psi_i(\xi)$ Polynomials from Askey-Wiener scheme depending on ξ
- $< \psi_i \, \psi_j >= \delta_{ij}$ as before
- Galerkin Projection

Example

$$Y(x, t\xi) = \sum_{i=0}^{1} Y_i(x, t)\psi_i(\xi)$$
$$= Y_0 + Y_1\xi$$
$$Y \sim N(Y_0, Y_1^2)$$

Independent of PDE

Example Contd.

$$Y_t + C\frac{\partial Y}{\partial t} = 0, \quad 0 \leq x \leq 1$$
$$Y(x, T) = Y_\phi(x - ct)$$
$$Y(x, t = 0, \xi) = g(\xi)cos(x)$$

Solution

$$Y(x, t) = g(\xi)cos(x - ct)$$

Contd.

Letting

$$Y(x,t,\xi) = \sum_{i=0}^{3} y_i(x,t)\psi_i(\xi)$$

$\psi_0 = 1$, $\psi_1 = \xi$, $\psi_2 = \xi^2 - 1$, $\psi_3 = \xi^3 - 3\xi$

$$\sum_{i=1}^{3} \frac{\partial Y_i}{\partial t}\psi_i(\xi) + c\sum_{i=0}^{s} \frac{\partial Y_i}{\partial x}\psi_i(\xi) = 0$$

How to solve?

Galerkin Projection

$$\int_{\xi} \sum_{i=0}^{3} \frac{\partial Y_i}{\partial t} \psi_i(\xi)\psi_j(\xi) w(\xi) d\xi + \int_{\xi} c \sum_{i=0}^{3} \frac{\partial Y_i}{\partial x} \psi_i(\xi)\psi_j(\xi) w(\xi) d\xi$$

Galerkin Projection Contd.

Simplifying

$$\sum_{i=0}^{3} \frac{\partial Y_i}{\partial t} \int_{\xi} \psi_i(\xi)\psi_j(\xi)w(\xi)d\xi$$

$$c\sum_{i=0}^{3} \frac{\partial Y_i}{\partial x} \int_{\xi} \psi_i(\xi)\psi_j(\xi)w(\xi)d\xi$$

This must be recognizable!

Galerkin Projection Contd.

$$\sum_{i=1}^{3} \frac{\partial Y_i}{\partial t} < \psi_i, \psi_j > + \sum_{i=1}^{3} \frac{\partial Y_i}{\partial x} < \psi_i, \psi_j >= 0$$

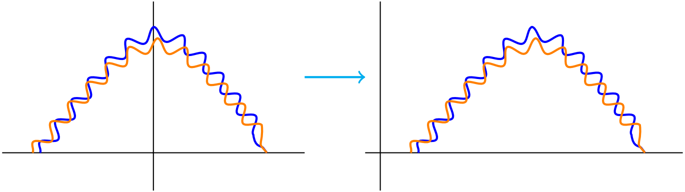
$$< \psi_i, \psi_j >= \delta_{ij}$$

$$\frac{\partial Y_0}{\partial t} + c\frac{\partial Y_0}{\partial x} = 0 \qquad \frac{\partial y_2}{\partial t} + \frac{\partial Y_2}{\partial x} = 0$$

$$\frac{\partial Y_1}{\partial t} + c\frac{\partial Y_1}{\partial x} = 0 \qquad \frac{\partial y_3}{\partial t} + \frac{\partial Y_3}{\partial x} = 0$$

Contd.

Uncoupled!



What ICs?

$$
\begin{aligned}
Y_0^{(\phi)} &= \int \cos(x) g(\xi) \psi^{(0)}(\xi) d\xi \\
&= \left\langle g(\xi),\, \psi^{(0)}(\xi) \right\rangle \cos(x) \\
Y_1^{(\phi)} &= \left\langle g_\varphi,\, \psi^{(1)} \right\rangle \cos(x) \\
Y_2^{(\phi)} &= \left\langle g_\varphi,\, \psi^{(2)} \right\rangle \cos(x) \\
Y_3^{(\phi)} &= \left\langle g_\varphi,\, \psi^{(3)} \right\rangle \cos(x)
\end{aligned}
$$

Could life be that simple!

Let's say

$$\frac{\partial Y}{\partial t} + c\frac{\partial Y}{\partial x} = 0$$

$$\begin{aligned} c &= g(\xi) \\ &= \sum_{i=0}^{N} g_j \psi_j(\xi) \quad (say) \end{aligned}$$

Repeating

$$\sum_{i=0}^{N} \frac{\partial Y_i}{\partial t} + c \sum_{i=0}^{N} \frac{\partial Y_i}{\partial x} \psi_i = 0$$

$$\downarrow$$

$$\sum_{i=0}^{N} \frac{\partial Y_i}{\partial t} \langle \psi_i, \psi_j \rangle + \sum_{i=0}^{N} \frac{\partial Y_i}{\partial x} \left\langle \psi_i \left(\sum_{k=1}^{N} g_k \psi_k \right) \psi_j \right\rangle = 0$$

$$= \sum_{i=0}^{N} \frac{\partial Y_i}{\partial t} \langle \psi_i, \psi_j \rangle + \sum_{i=0}^{N} \frac{\partial Y_i}{\partial x} \sum_{k=1}^{N} g_k \langle \psi_i \, \psi_j \, \psi_k \rangle = 0$$

Tough!

N+1 Coupled Equations!
Need to totally change code
Intrusive $\Leftrightarrow$Stochastic Galerkin scheme.

Summary

Many ways to propagate uncertainty

- Monte-Carlo
- PCM/SCM/RSM
- PC/gPC
- MOR/POD etc

There are others:
e.g. using wavelets instead of polynomials
Much work to do!

Key Topics

1. Non Gaussian distributions
2. Non intrusive methodology
3. Non linearity
4. Fast computation

Methodology is very much “open”