(Generalized) Polynomial Chaos representation

Didier Lucor

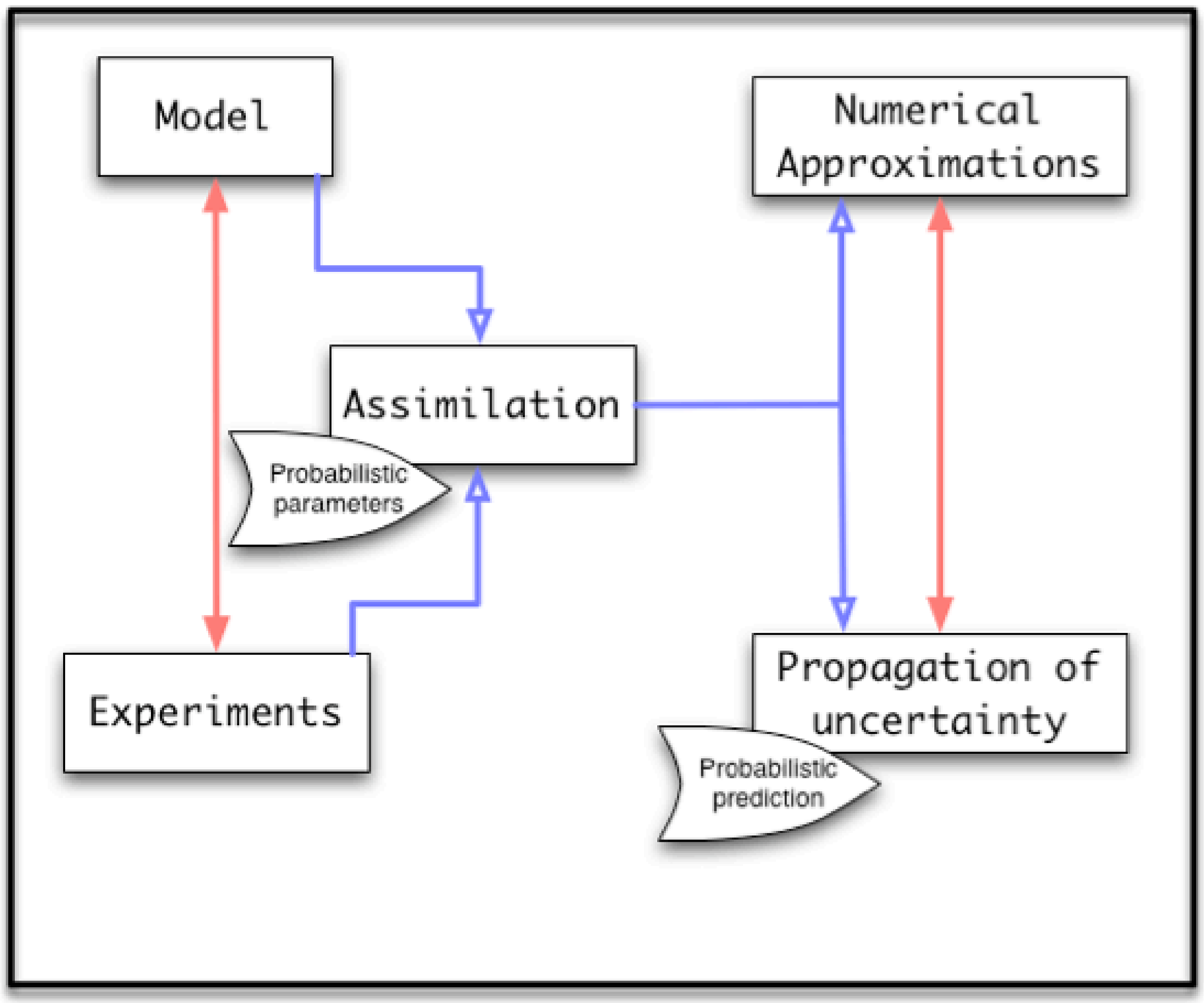
Laboratoire de Modélisation en Mécanique

UPMC Paris VI www.lmm.jussieu.fr

Outline

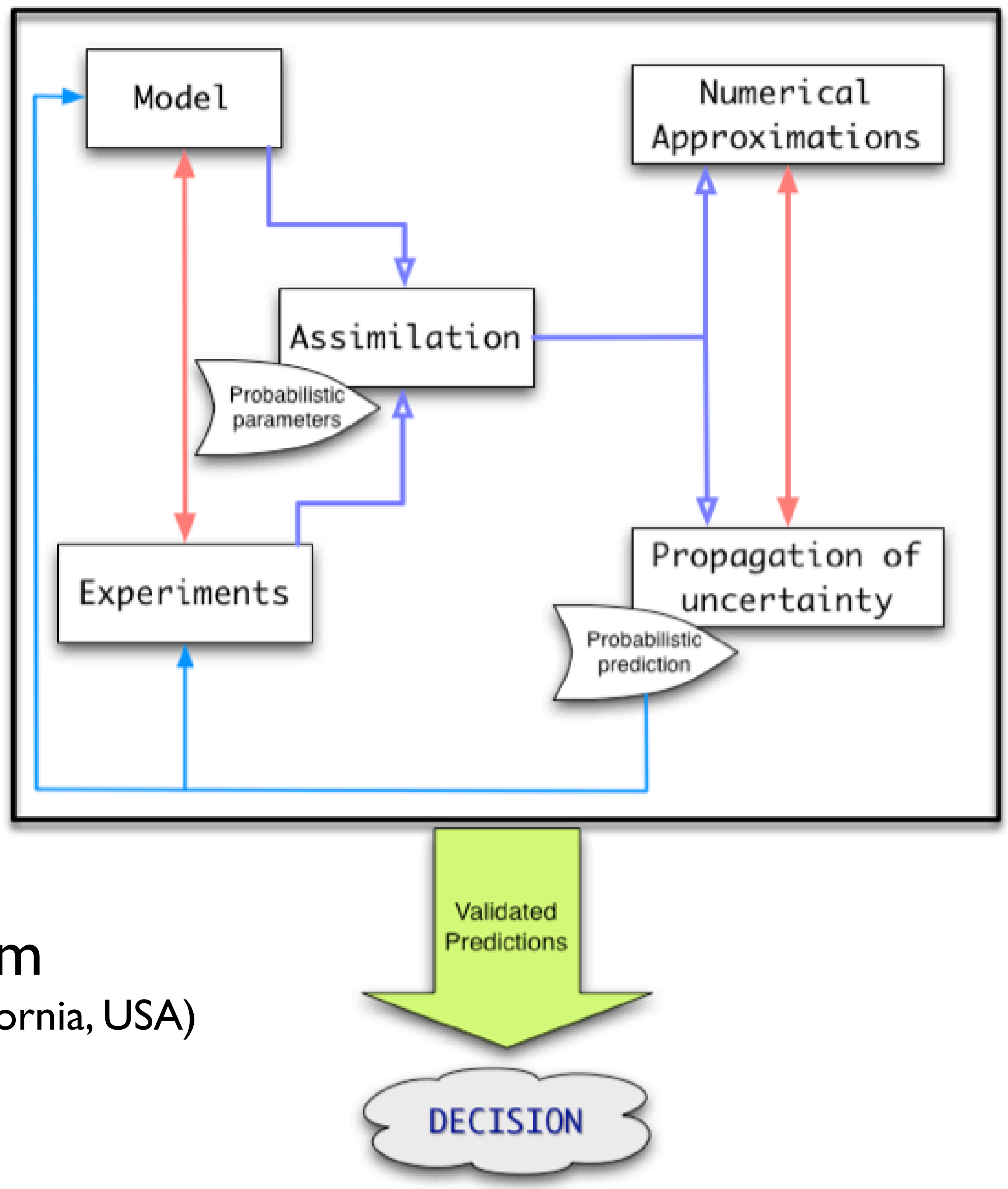
- Context & Motivation
- Polynomial Chaos and generalized Polynomial Chaos Expansions
- Limitations & Difficulties of the method
- Possible applications

Interaction of model and data



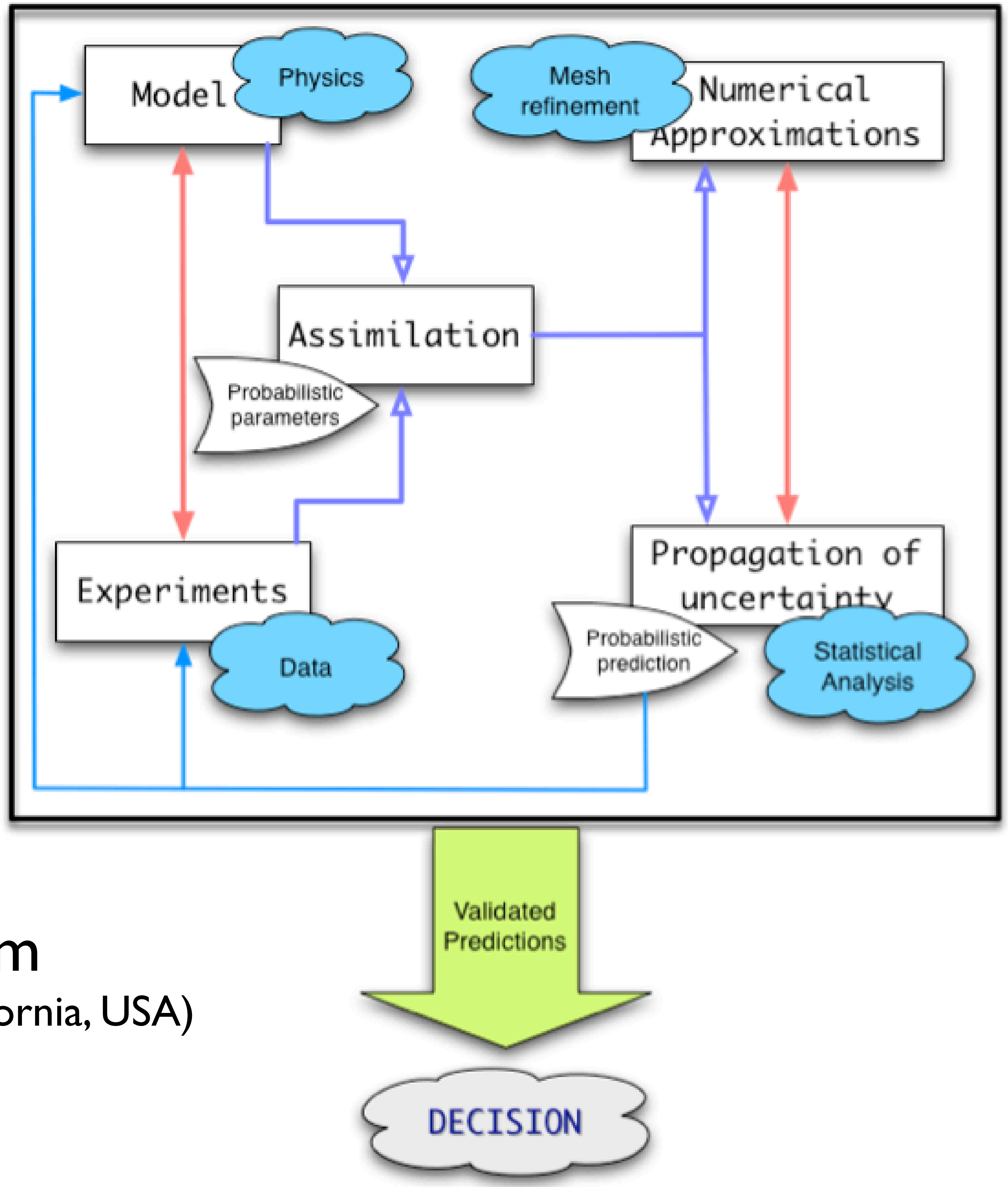
Roger Ghanem
(University of Southern California, USA)

Interaction of model and data



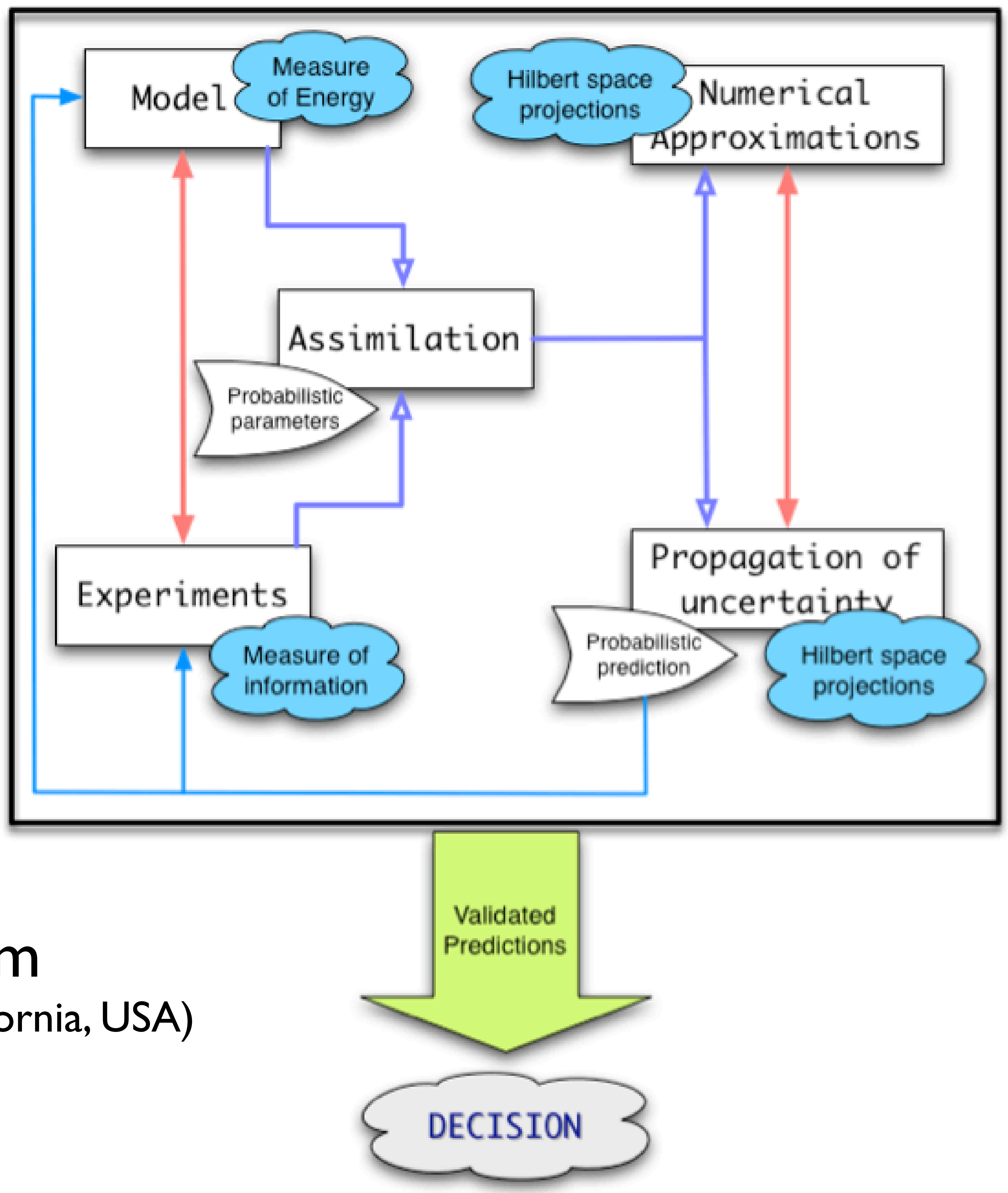
Roger Ghanem
(University of Southern California, USA)

Interaction of model and data



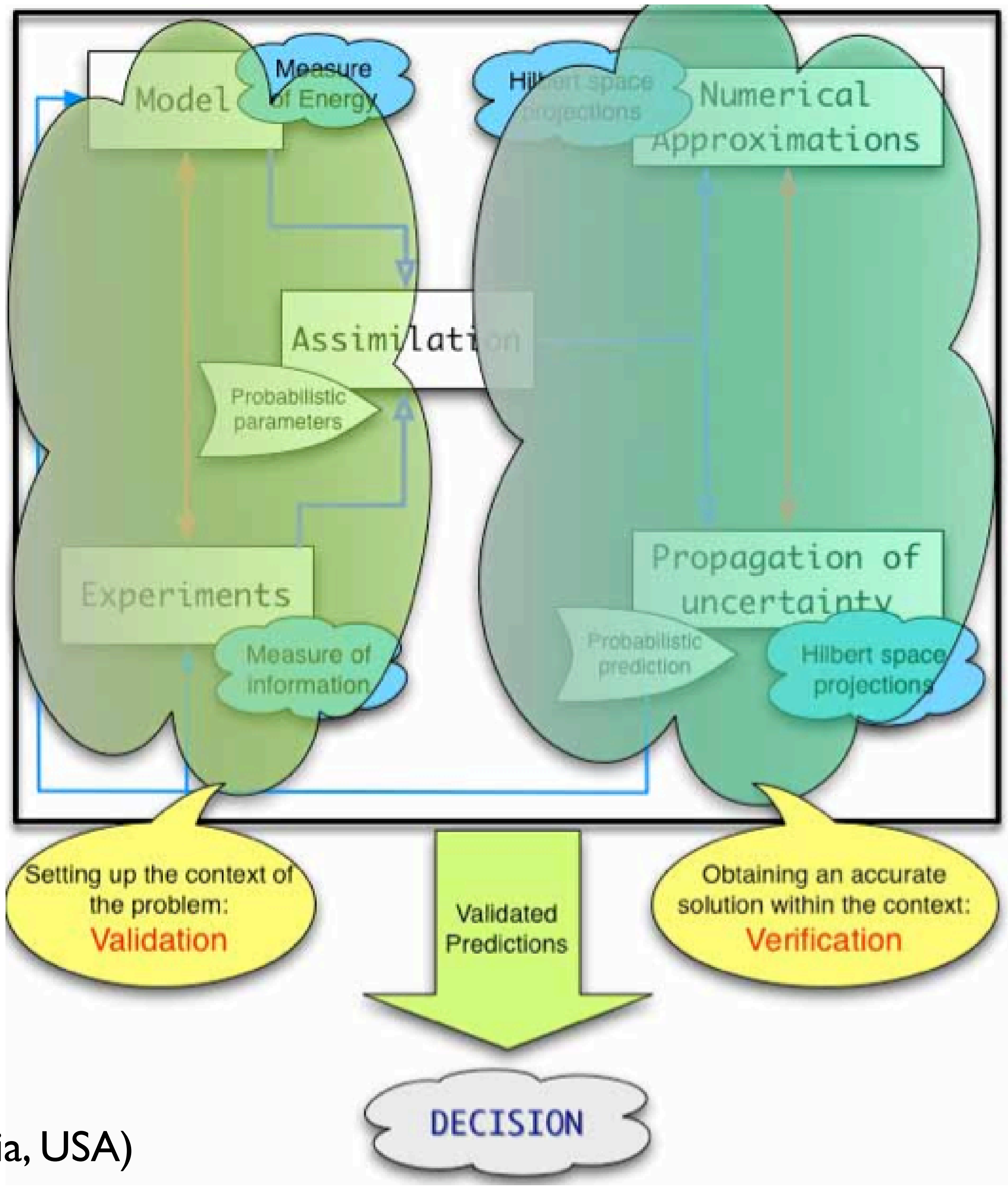
Roger Ghanem
(University of Southern California, USA)

Interaction of model and data



Roger Ghanem
(University of Southern California, USA)

Interaction of model and data

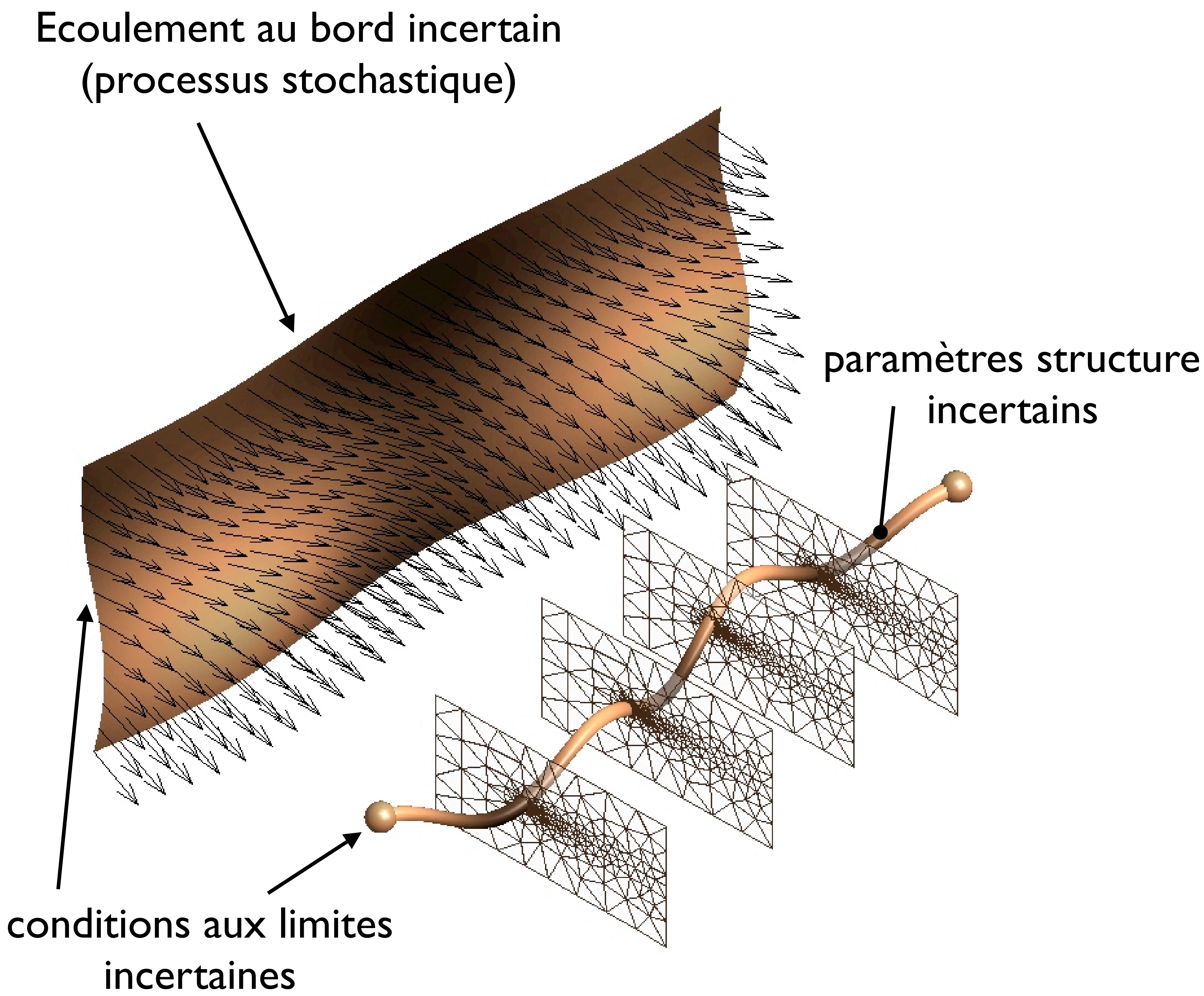


Roger Ghanem
(University of Southern California, USA)

Uncertainty Quantification (UQ)

- Modeling errors/uncertainties, numerical errors and data errors/uncertainties can interact. This brings the need for uncertainty quantification.
- Need to access the impact of uncertain data on simulation outputs.
- In case of the lack of a reference solution, the validity of the model can be established only if uncertainty in numerical predictions due to uncertain input parameters can be quantified.
- Difficulty: instead of looking for the *unique* solution of a single deterministic problem, one is now interested in finding and parameterizing the space of *all possible* solutions spanned by the uncertain parameters.

Sources d’incertitudes



- paramètres/constantes de simulation, conditions d'opération
- coefficients de transport, propriétés physiques
- géométrie
- conditions aux bords, conditions initiales
- lois de comportement, schéma numériques

Représentation des Processus Aléatoires

Méthodes statistiques (non déterministes)

- Monte-Carlo: convergence en $1/\sqrt{N}$, taux de convergence ne depends pas du nombre de variables aleatoires.
- Monte-Carlo et ses variantes: tirages descriptifs, hypercube, optimal Latin hypercube (Latin Hypercube Sampling, Quasi-Monte Carlo [QMC] method, Markov Chain Monte Carlo method [MCMC], importance sampling, correlated sampling, conditional sampling, Variance reduction technique, Response Surface Method [RSM]).

Méthodes non-statistiques (directes)

- Développement en séries de Taylor ou méthode des perturbations (1er ou 2nd ordre).
- Méthode itérative ou séries de Neumann et méthode d'intégrale pondérée.
- Méthode spectrale et méthode de développements orthogonaux: Polynômes de Chaos (PC-Chaos Homogène-Chaos Hermite, Generalized Polynomial Chaos [gPC]-Chaos Askey), expansion de Karhunen Loève.

Wiener, *The homogeneous chaos*, Amer. J. Math., 60 (1938).
Ghanem & Spanos, *Stochastic Finite Elements: a Spectral Approach*, Springer-Verlag, (1991).
Loève, *Probability Theory*, Fourth edition, Springer-Verlag, (1977).

Modélisation spectrale de l'incertitude

- **Concept:**

  Approche probabiliste qui considère que l'incertitude génère de nouvelles dimensions et que la solution dépend de ces dimensions.

  Représentation de la solution sous forme d'expansion convergente construite grâce à une projection sur une base spectrale; les coefficients sont calculés par le biais de projections.

- **Avantages:**

  Mesure efficace de la sensibilité de la solution aux paramètres d'entrée incertains

  Obtention d'une forme explicite de la solution + moments + PDF

- **Applications:**

  Mécanique des structures élastiques stochastiques, écoulement en milieu poreux, équations de Navier-Stokes, problèmes thermiques, combustion et fluides réactifs, séismologie, micro-fluides et électrochimie.

Polynômes de Chaos (Wiener 1938)

Soit l'espace probabilisé: $(\Omega, \mathcal{A}, \mathcal{P})$

Event space

σ-algebra of ***Ω***

Probability measure

$X : \Omega \to V$ Processus stochastique du second ordre si:

$X(\omega)$ peut s'exprimer en fonction de $\{\xi_j(\omega)\}_{j=1}^{N}$ avec $\omega \in \Omega$ et $N \in \mathbb{N}$

$$\mathbb{E}\|X\|^2 = \mathbb{E}(X, X) < \infty$$

$$\mathbb{E}Y = \int_{\omega\in\Omega} Y(\omega) dP(\omega) \qquad Y \in L^1(\Omega, \mathbb{R})$$

$$\begin{aligned} X(\omega) &= a_0\Phi_0 + \sum_{i_1=1}^{\infty} a_{i_1}\Phi_1(\xi_{i_1}(\omega)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} a_{i_1 i_2}\Phi_2(\xi_{i_1}(\omega), \xi_{i_2}(\omega)) \\ &+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}\Phi_3(\xi_{i_1}(\omega), \xi_{i_2}(\omega), \xi_{i_3}(\omega)) \\ &+ \cdots, \end{aligned}$$

Theoreme de Cameron & Martin (1947):
PC-homogène converge pour toute fonctionnelle de L_2

Polynômes de Chaos (continued)

$$X(\omega) = \sum_{k=0}^{\infty} a_k \Phi_k(\boldsymbol{\xi}(\omega))$$

- Spectral expansion on orthogonal (*in the mean sense* $<\Phi_i\,,\Phi_j>=0$ if $i\neq j$) ***Hermite*** polynomial basis Φ_k.
- ξ is here a "random array" of independent ***Gaussian*** random variables of the random event ω.
- Once computed, the knowledge of the coefficients a_k fully determines the random process $X(\omega)$.
- This concept can be generalized to other non-normal measures.

Polynômes de Chaos (truncated form)

$$\boxed{X(\boldsymbol{x},t,\boldsymbol{\xi}) = X(\boldsymbol{x},t,\xi_1,\xi_2,\ldots\xi_N) \approx \sum_{j=0}^{M} X_j(\boldsymbol{x},t)\Phi_j(\boldsymbol{\xi})}$$

$$(M+1) = (N+P)!/(N!P!)$$

$$\nu = \{\Phi_j, j = 0,\ldots,M\}$$

- is the set of vectors spanning the process and the orthogonal basis Φ_j is a set of polynomials with degree at most equal to P.
- The orthogonality relation gives:

$$< \Phi_i(\xi), \Phi_j(\xi) >= \int_{-\infty}^{\infty} \Phi_i(\xi)\Phi_j(\xi)d\xi = 0 \ \text{ if } \ i \neq j$$

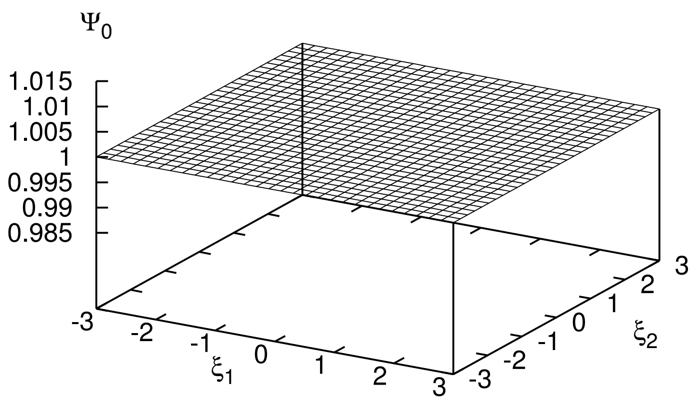
with the inner product defined as: $$\langle f(\boldsymbol{\xi})g(\boldsymbol{\xi})\rangle = \int_{\omega\in\Omega} f(\boldsymbol{\xi})g(\boldsymbol{\xi})dP(\omega) = \int f(\boldsymbol{\xi})g(\boldsymbol{\xi})w(\boldsymbol{\xi})d\boldsymbol{\xi}$$

Example of multi-dimensional homogeneous PC expansion

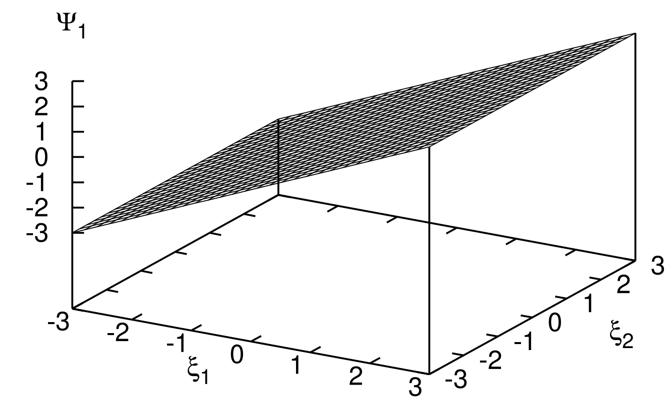
$$\{\xi_j(\omega)\}_{j=1}^{N} \quad \text{here } N=2 \longrightarrow \boldsymbol{\xi} := \{\xi_j(\omega)\}_{j=1}^{N} = \{\xi_1, \xi_2\}$$

The weight function is: $$w(\xi_1,\xi_2) = \frac{1}{2\pi}\exp^{-\xi_1^2/2}\ \exp^{-\xi_2^2/2}$$

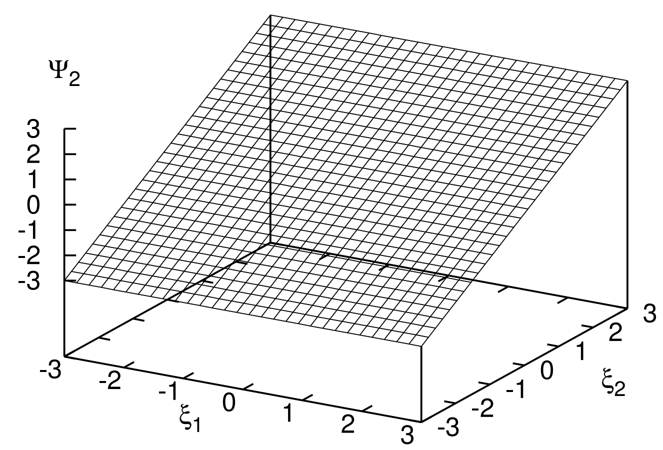
Zero & 1st order **Hermite** polynomials



$$\Psi_0 = 1$$

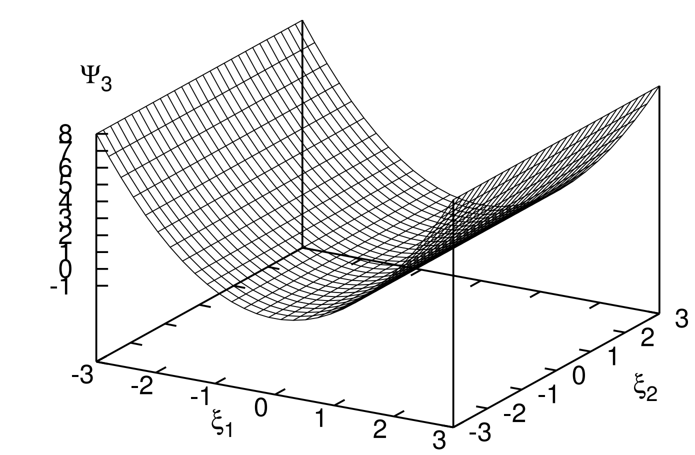


$$\Psi_1 = \xi_1$$

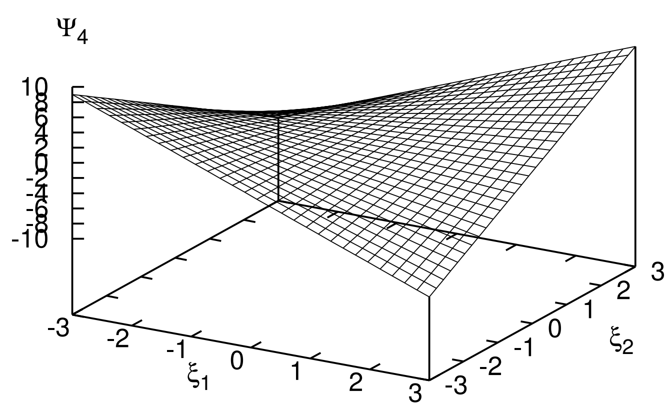


$$\Psi_2 = \xi_2$$

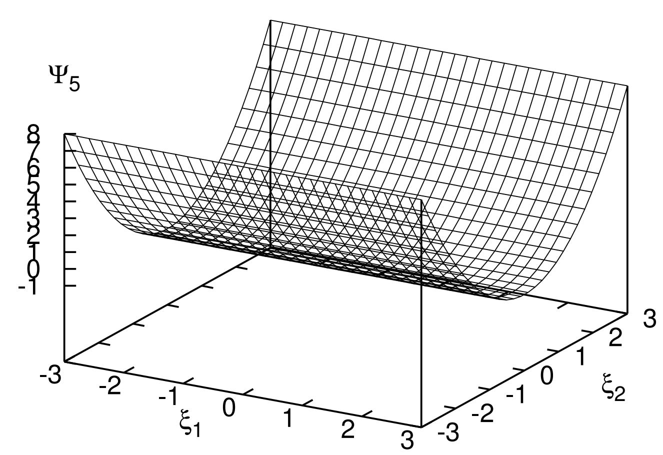
2nd order **Hermite** polynomials



$$\Psi_3 = \xi_1^2 - 1$$



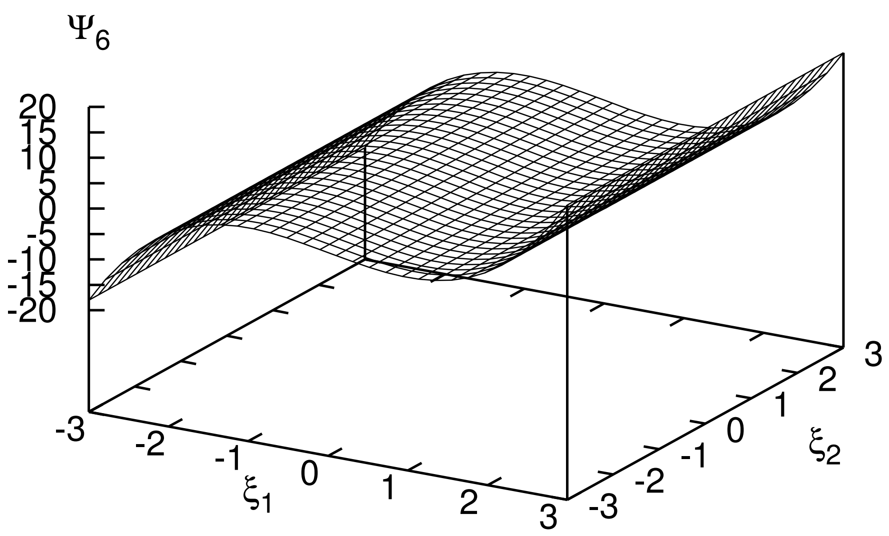
$$\Psi_4 = \xi_1\xi_2$$



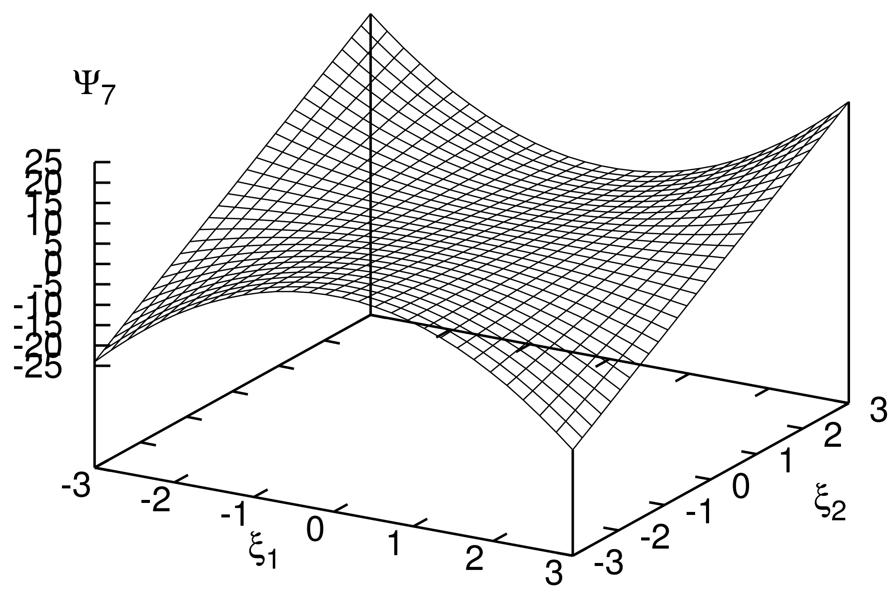
$$\Psi_5 = \xi_2^2 - 1$$

Example of multi-dimensional homogeneous PC expansion

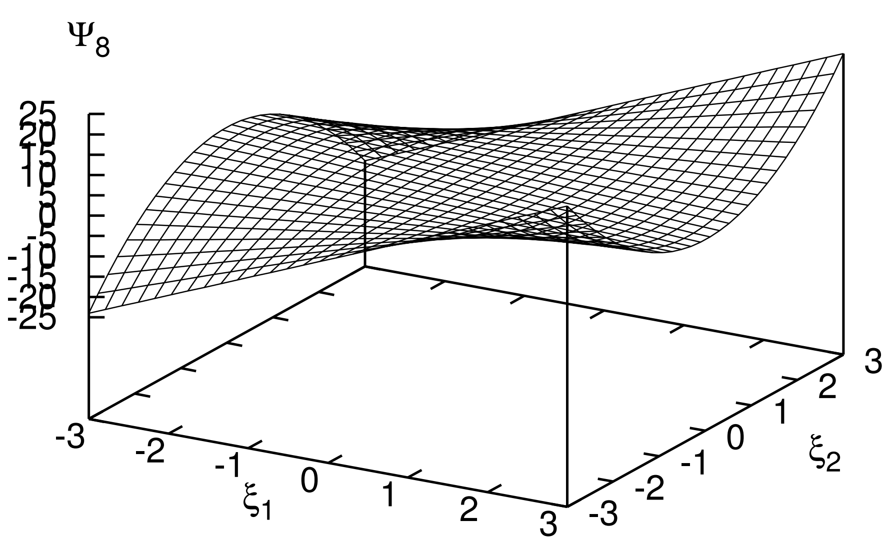
3rd order **Hermite** polynomials



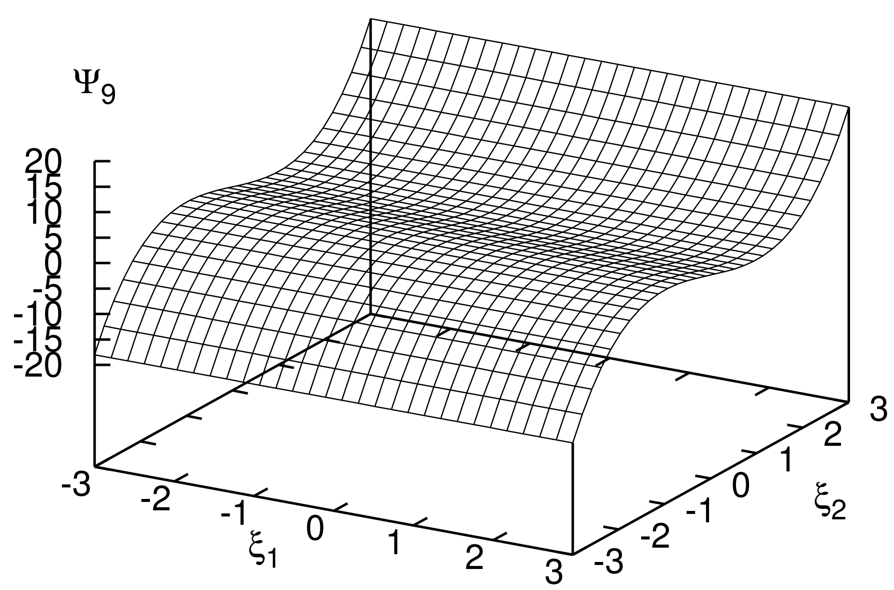
$$\Psi_6 = \xi_1^3 - \xi_1$$



$$\Psi_7 = \xi_1^2 \xi_2 - \xi_2$$



$$\Psi_8 = \xi_1 \xi_2^2 - \xi_1$$

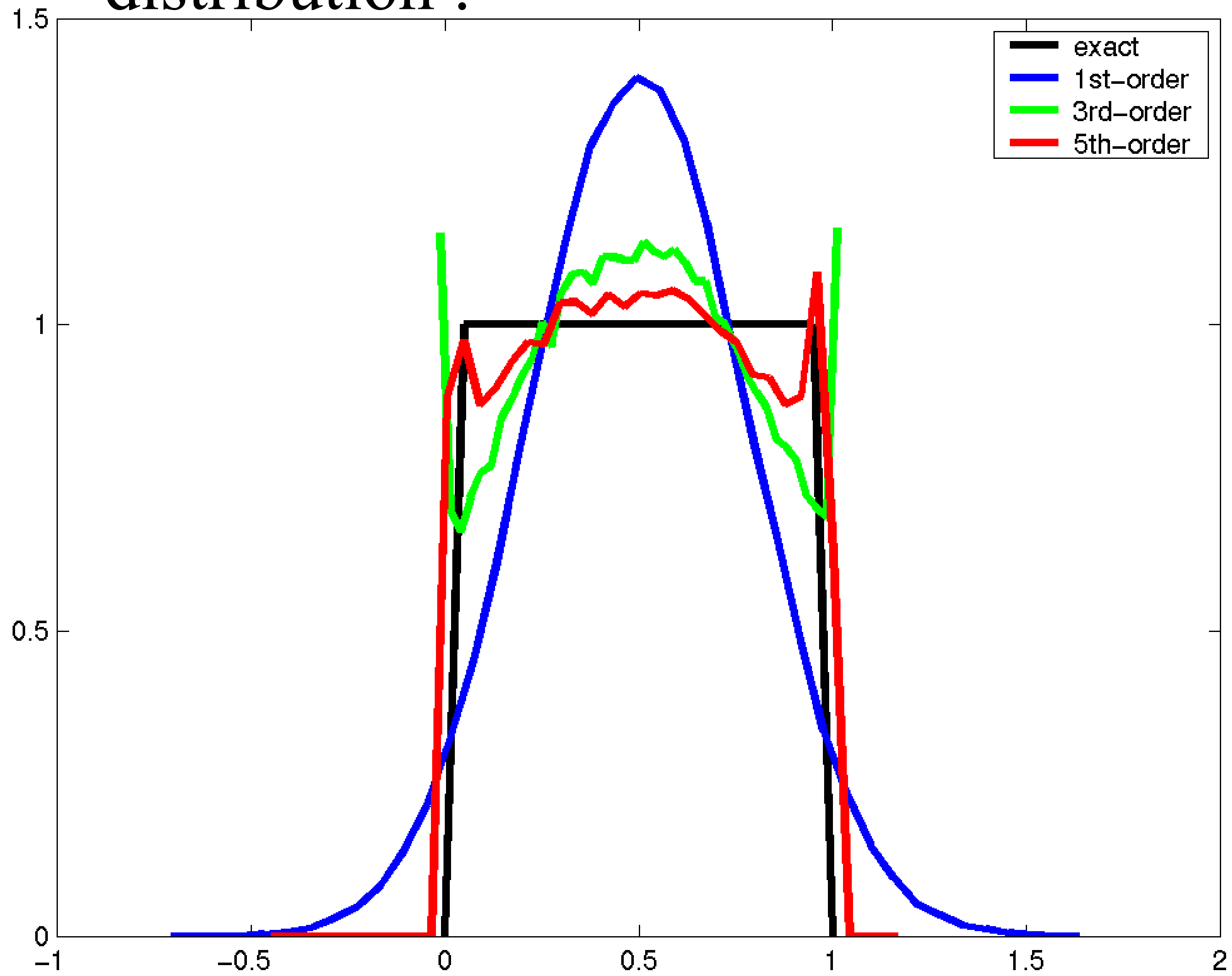


$$\Psi_9 = \xi_2^3 - \xi_2$$

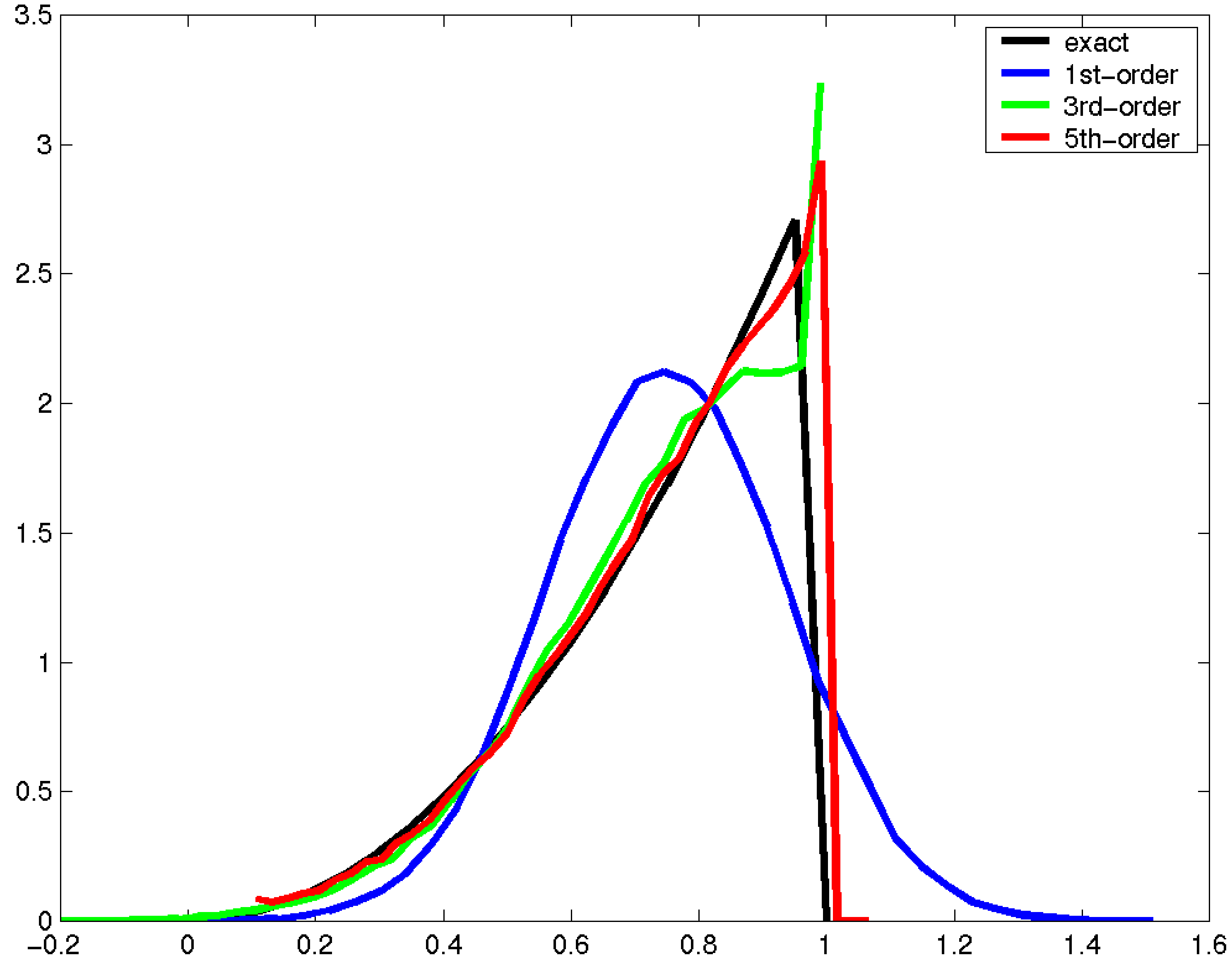
Hermite-Chaos Expansion of Beta Distribution

$$\text{PDF}: \quad f(x) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}, \quad \alpha,\beta > 0, \quad 0 \le x \le 1$$

Uniform distribution : $\alpha = 1, \quad \beta = 1$



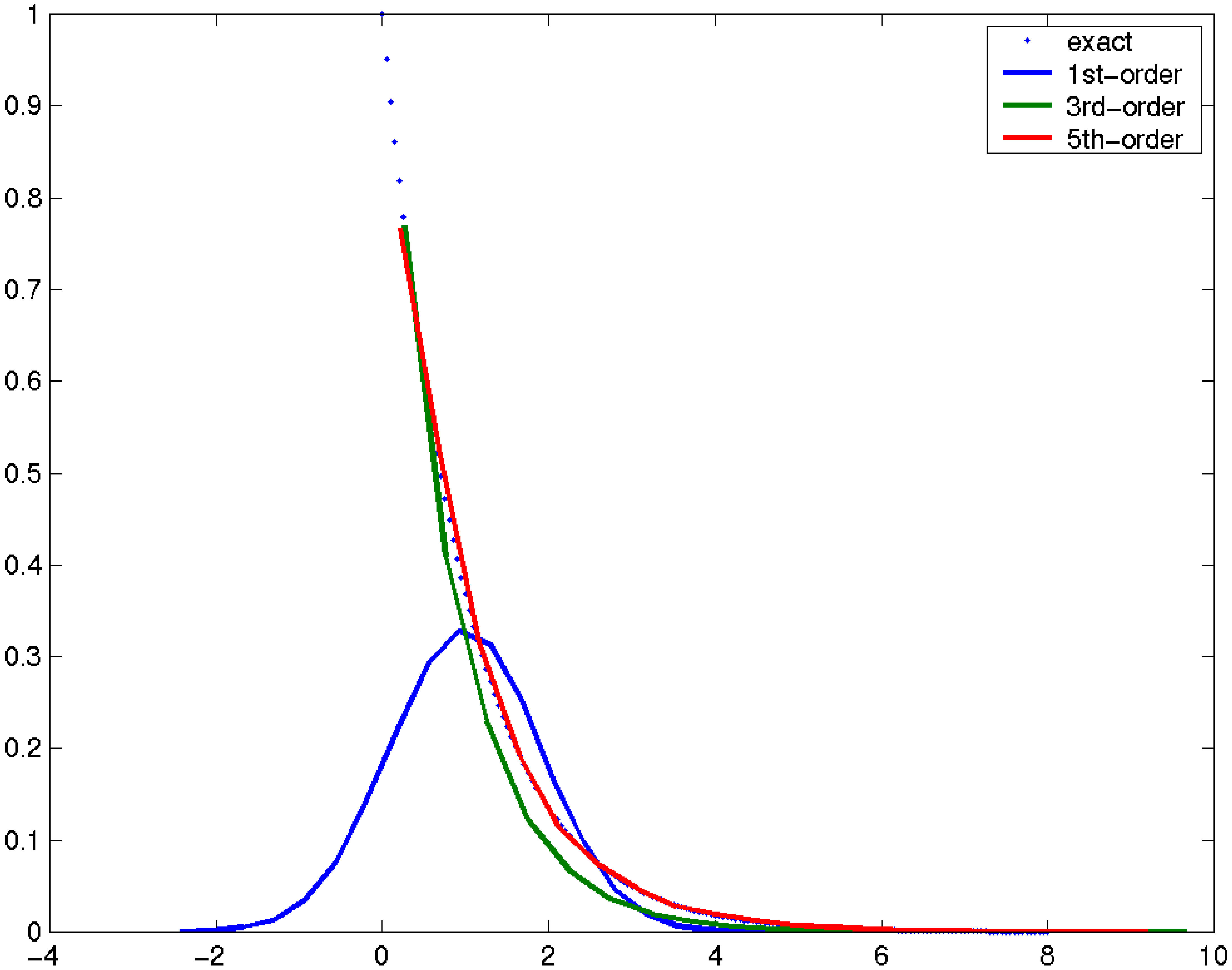
$\alpha = 3, \quad \beta = 1$



Exact PDF and PDF of 1st, 3rd, 5th-order Hermite-Chaos Expansions

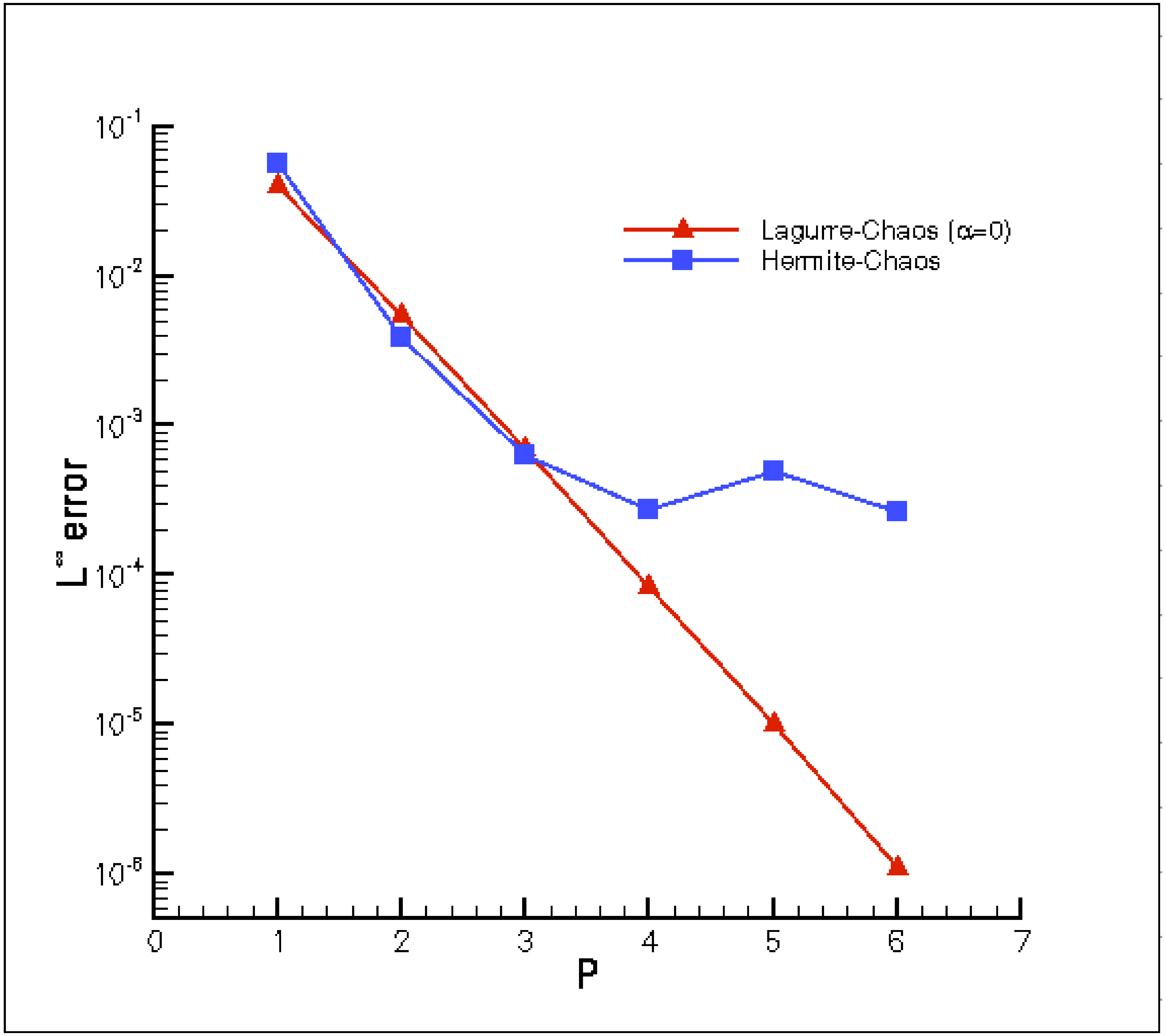
Hermite-Chaos Expansion of Gamma Distribution

$$\text{PDF}: \quad f(x) = \frac{e^{-x} x^{\alpha-1}}{\Gamma(\alpha)}, \quad \alpha > 0, \quad x \ge 0. \qquad \alpha = 1\text{: exponential distribution}$$



PDF of exponential distribution and 1st, 3rd and 5th-order Hermite-Chaos

Exponential Input: Laguerre (optimal) vs. Hermite



Convergence w.r.t. number of expansion terms

Polynômes de Chaos (Généralisés)

Représentation spectrale d'un processus stochastique du second ordre:

$$X(\omega) = \sum_{k=0}^{\infty} a_k \Phi_k(\boldsymbol{\xi}(\omega))$$

$\boldsymbol{\xi} := \{\xi_j(\omega)\}_{j=1}^{N}$ n'est **pas** limité à une distribution gaussienne!

$$\langle \Phi_i \Phi_j \rangle = \langle \Phi_i^2 \rangle \delta_{ij}$$

produit interne: $\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \int_{\omega \in \Omega} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) dP(\omega) = \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi}$

$$\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \sum_{\boldsymbol{\xi}} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi})$$

Polynômes de Chaos (Généralisés)

Coefficients spectraux **déterministes** à calculer et qui déterminent complètement le processus

$$X(\omega) = \sum_{k=0}^{\infty} \boxed{a_k} \Phi_k(\boldsymbol{\xi}(\omega))$$

$\boldsymbol{\xi} := \{\xi_j(\omega)\}_{j=1}^{N}$ n'est **pas** limité à une distribution gaussienne!

$$\langle \Phi_i \Phi_j \rangle = \langle \Phi_i^2 \rangle \delta_{ij}$$

produit interne: $\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \int_{\omega \in \Omega} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) dP(\omega) = \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi}$

$$\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \sum_{\boldsymbol{\xi}} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi})$$

Polynômes de Chaos (Généralisés)

$$X(\omega) = \sum_{k=0}^{\infty} a_k \Phi_k(\boldsymbol{\xi}(\omega))$$

Fonctions **orthogonales**
(trigonométriques, wavelets,... polynômes)

$\boldsymbol{\xi} := \{\xi_j(\omega)\}_{j=1}^{N}$ n'est **pas** limité à une distribution gaussienne!

$$\boxed{\langle \Phi_i \Phi_j \rangle = \langle \Phi_i^2 \rangle \delta_{ij}}$$

produit interne: $\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \int_{\omega\in\Omega} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) dP(\omega) = \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi}$

$$\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \sum_{\boldsymbol{\xi}} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi})$$

Polynômes de Chaos (Généralisés)

$$X(\omega) = \sum_{k=0}^{\infty} a_k \Phi_k(\boxed{\boldsymbol{\xi}}(\omega))$$

Variables aléatoires indépendantes

(distribution statistiques prescrites)

$$\boldsymbol{\xi} := \{\boxed{\xi_j}(\omega)\}_{j=1}^{N}$$

n'est **pas** limité à une distribution gaussienne!

$$\langle \Phi_i \Phi_j \rangle = \langle \Phi_i^2 \rangle \delta_{ij}$$

produit interne: $\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \int_{\omega \in \Omega} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) dP(\omega) = \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi}$

$$\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \sum_{\boldsymbol{\xi}} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi})$$

Polynômes de Chaos (Généralisés)

$$X(\omega) = \sum_{k=0}^{\infty} a_k \Phi_k(\boldsymbol{\xi}(\omega))$$

$\boldsymbol{\xi} := \{\xi_j(\omega)\}_{j=1}^{N}$ n'est **pas** limité à une distribution gaussienne!

Etroite correspondance entre la **fonction de poids** du polynôme choisi et la **densité de probabilité** de l'incertitude

produit interne: $\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \int_{\omega \in \Omega} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) dP(\omega) = \int f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi}$

$$\langle f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) \rangle = \sum_{\boldsymbol{\xi}} f(\boldsymbol{\xi}) g(\boldsymbol{\xi}) w(\boldsymbol{\xi})$$

Hypergeometric Orthogonal Polynomials

- Generalized hypergeometric series:

$$ {}_rF_s(a_1,\cdots,a_r;b_1,\cdots,b_s;z)=\sum_{j=0}^{\infty}\frac{(a_1)_j\cdots(a_r)_j}{(b_1)_j\cdots(b_s)_j}\frac{z^j}{j\;!},\quad b_i\neq 0,-1,-2,\cdots $$

- Pochhammer symbol: $(a)_n=\dfrac{\Gamma(a+n)}{\Gamma(a)}=\begin{cases}1, & \text{if } n=0,\\ a(a+1)\cdots(a+n-1), & \text{if } n=1,2,3,\dots\end{cases}$

- Infinite series converge under certain conditions: $\rho=\begin{Bmatrix}\infty, & r<s+1\\ 1, & r=s+1\\ 0, & r>s+1\end{Bmatrix}$

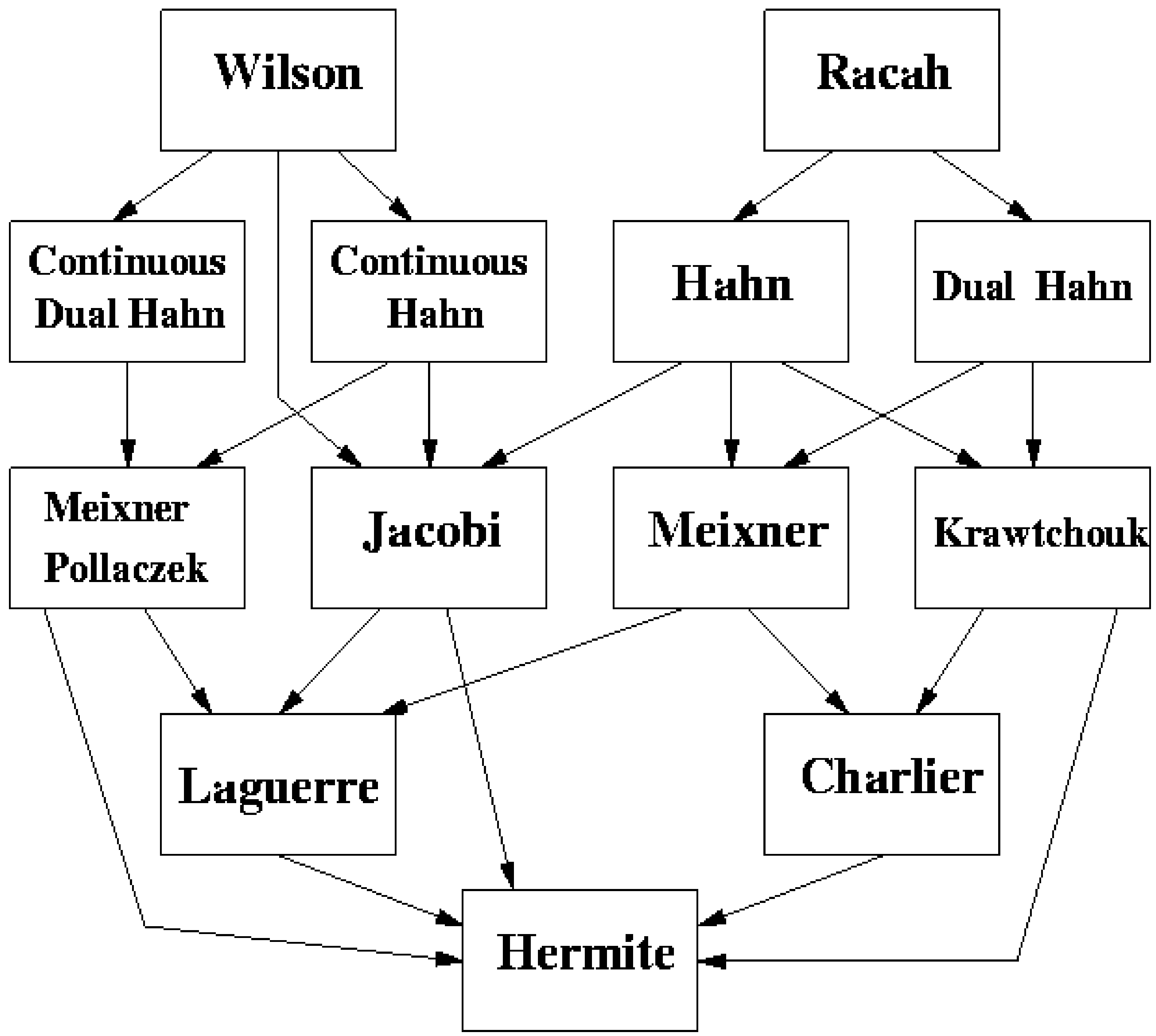
- Examples: ${}_0F_0$ is exponential series; ${}_1F_0$ is binomial series.

- If one of the a_i's is a negative integer ($-n$), the series terminate at $n^{\text{th-}}$term and become hypergeometric orthogonal polynomials:

$$ {}_rF_s(a_1,\cdots,a_r;b_1,\cdots,b_s;z)=\sum_{j=0}^{n}\frac{(-n)_j\cdots(a_r)_j}{(b_1)_j\cdots(b_s)_j}\frac{z^j}{j\;!},\quad b_i\neq 0,-1,-2,\cdots $$

- Limit relations: e.g. $\lim\limits_{\alpha\to\infty}\alpha^{-\frac{1}{2}n}P_n^{(\alpha,\alpha)}\left(\dfrac{x}{\sqrt{\alpha}}\right)=\dfrac{H_n(x)}{2^n n!}$

The Askey scheme of Hypergeometric Polynomials



Askey-scheme

Hypergeometric Orthogonal Polynomials

- Orthogonal polynomials $\{Q_n(x), n \in N\}$, $Q_n(x) = \sum_{k=0}^{n} a_k x^k$, $n \geq 0, a_n \neq 0.$
- Three-term recurrence: $Q_{n+1}(x) = (A_n x + B_n) Q_n(x) - C_n Q_{n-1}(x)$, $Q_{-1}(x) = 0$, $Q_0(x) = 1$, where $A_n, C_n \neq 0$, and $C_n A_n A_{n-1} > 0$.
- Favard's inverse theorem
- Orthogonality: $\int_x Q_n(x) Q_m(x) w(x) dx = h_n^2 \delta_{mn}$ $\sum_x Q_n(x) Q_m(x) w(x) = h_n^2 \delta_{mn}$
- Weighting functions and PDFs:
  - Continuous:

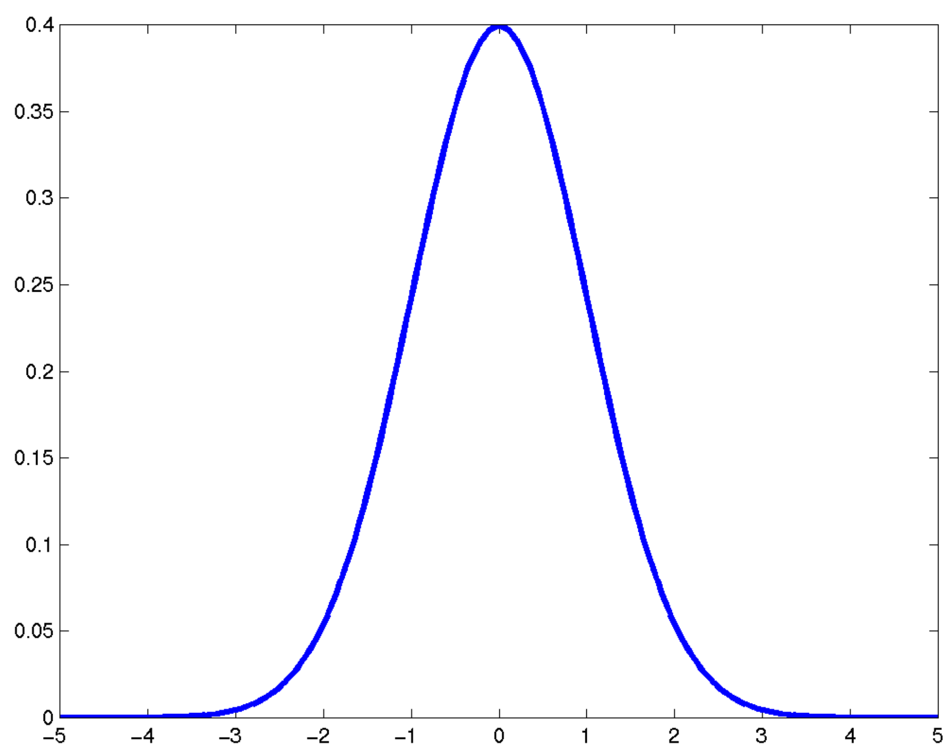
	Definition	Weighting function	PDF
Hermite	$(2x)^n {}_2F_0\left(-\frac{n}{2}, -\frac{n-1}{2}; ; -\frac{2}{x^2}\right)$	$\frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$	Gaussian
Laguerre	$\frac{(\alpha+1)_n}{n!} {}_1F_1(-n; \alpha+1; x)$	$\frac{x^\alpha e^{-x}}{\Gamma(\alpha+1)}$	Gamma
Jacobi	$\frac{(\alpha+1)_n}{n!} {}_2F_1\left(-n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2}\right)$	$\frac{2^{-(\alpha+\beta+1)}}{B(\alpha+1, \beta+1)} (1-x)^\alpha (1+x)^\beta$	Beta

  - Discrete:

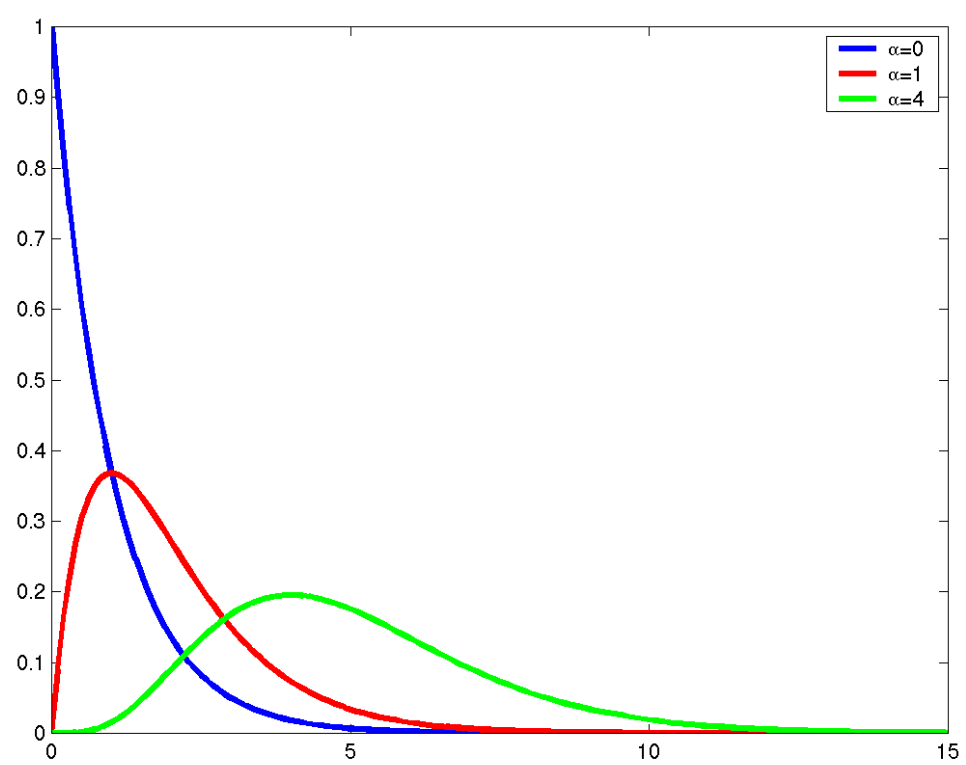
	Definition	Weighting function	PDF
Charlier	${}_2F_0(-n, -x; ; -1/a)$	$a^x / x!$	Poisson
Krawtchouk	${}_2F_1\left(-n, -x; -N; \frac{1}{p}\right)$	$\binom{N}{x} p^x (1-p)^{N-x}, 0 < p < 1$	Binomial
Meixner	${}_2F_1\left(-n, -x; \beta; 1-\frac{1}{c}\right)$	$\frac{(\beta)_x}{x!} (1-c)^\beta c^x, \beta > 0, 0 < c < 1$	Negative Bionomial
Hahn	${}_3F_2(\cdots)$	---	Hypergeometric

Orthogonal Polynomials and Probability Distributions

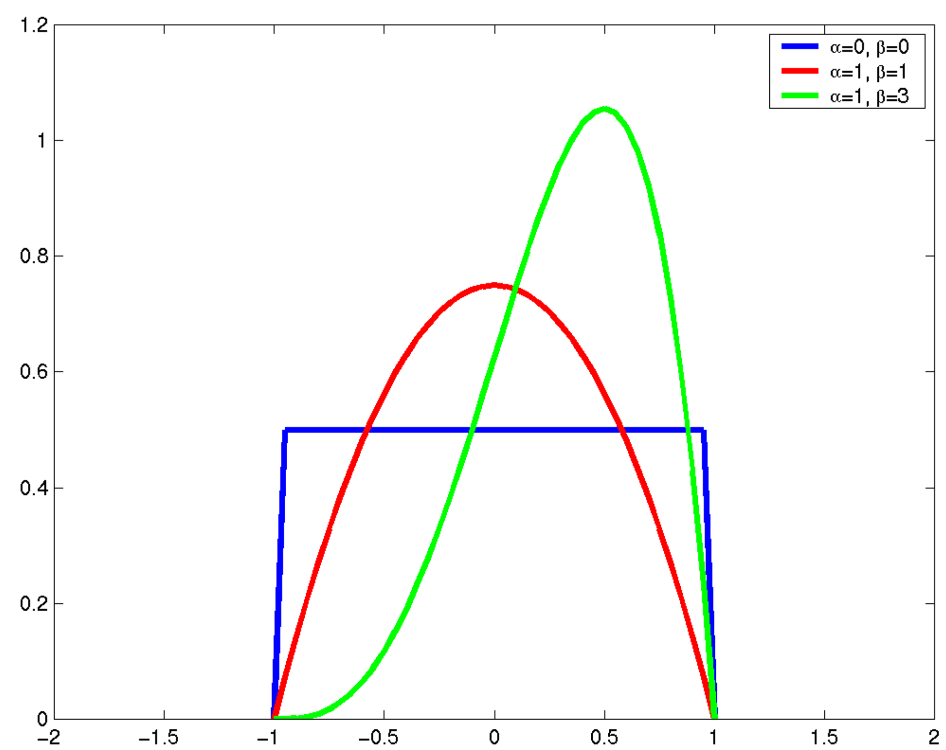
- **Continuous Cases**:
  - *Hermite* Polynomials $\longleftrightarrow$ *Gaussian* Distribution
  - *Laguerre* Polynomials $\longleftrightarrow$ *Gamma* Distribution
    (special case: *exponential* distribution)
  - *Jacobi* Polynomials $\longleftrightarrow$ *Beta* Distribution
  - *Legendre* Polynomials $\longleftrightarrow$ *Uniform* Distribution



Gaussian
distribution



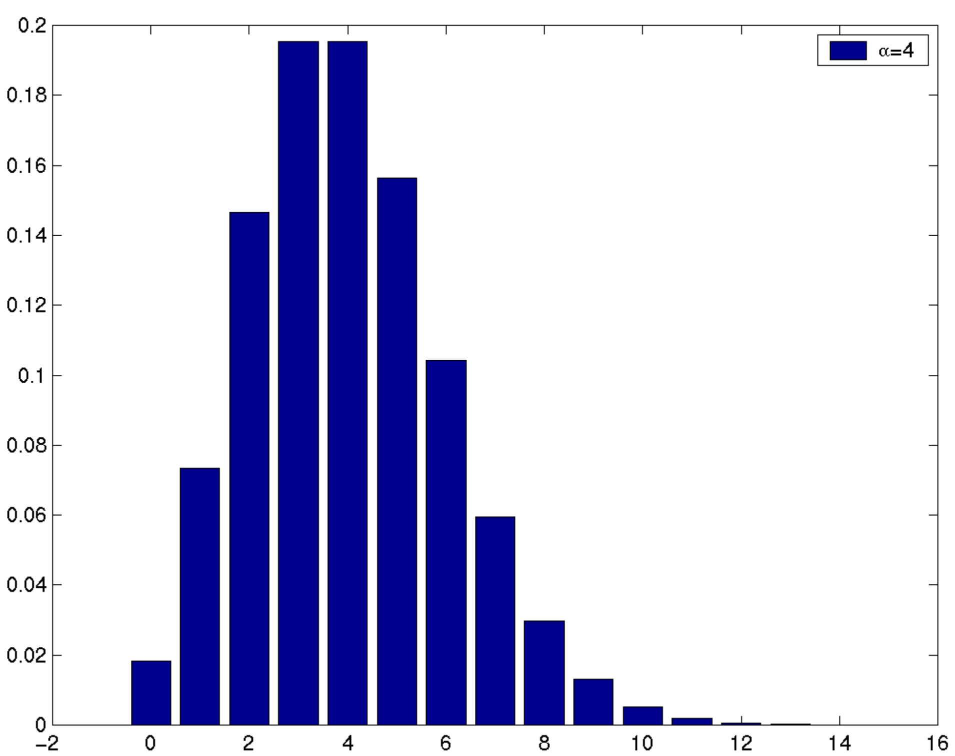
Gamma
distribution



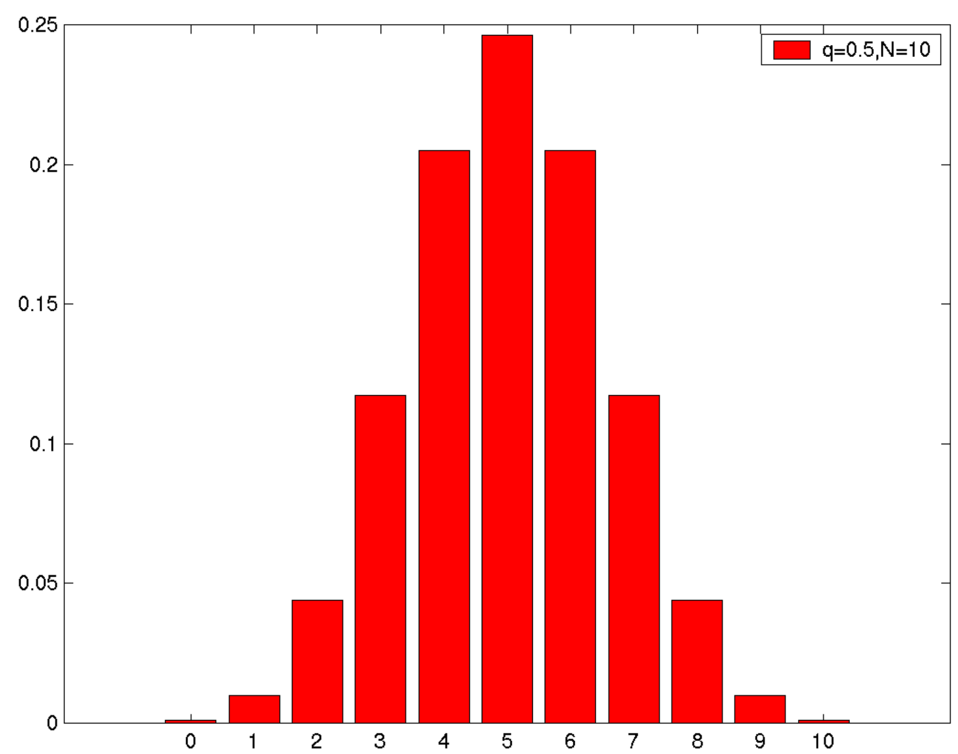
Beta
distribution

Orthogonal Polynomials and Probability Distributions

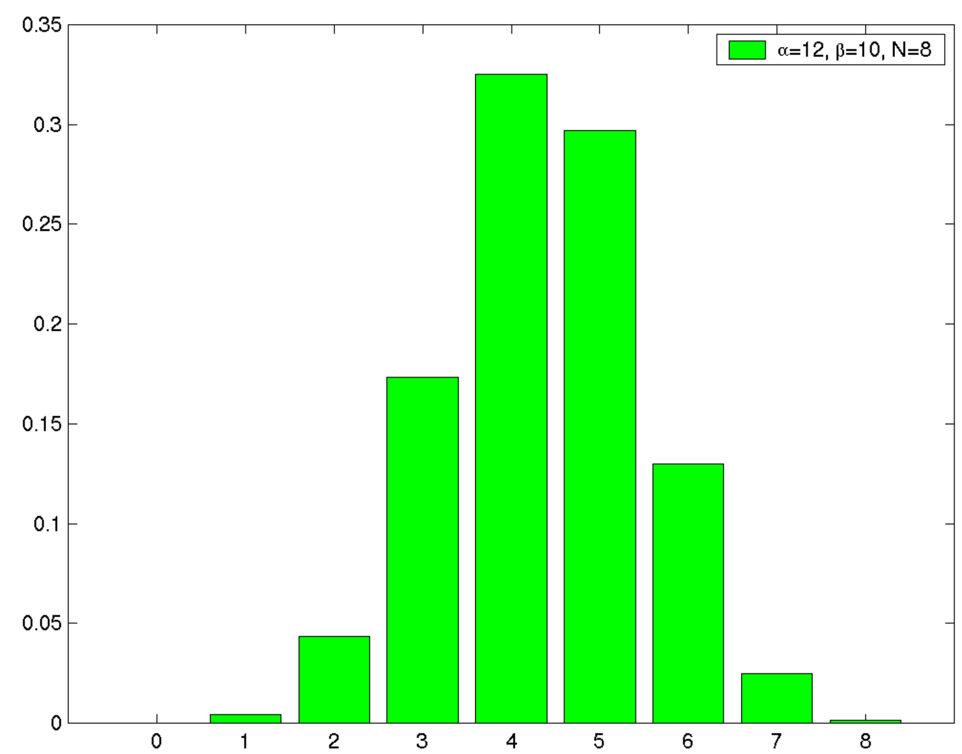
- **Discrete Cases :**
  - *Charlier* Polynomials ⟷ *Poisson* Distribution
  - *Krawtchouk* Polynomials ⟷ *Binomial* Distribution
  - *Hahn* Polynomials ⟷ *Hypergeometric* Distribution
  - *Meixner* Polynomials ⟷ *Pascal* Distribution



Poisson distribution



Binomial distribution



Hypergeometric distribution

Polynômes de Chaos (Résumé)

$$\boxed{X(\boldsymbol{x},t,\boldsymbol{\xi}) = X(\boldsymbol{x},t,\xi_1,\xi_2,\ldots\xi_N) \approx \sum_{j=0}^{M} X_j(\boldsymbol{x},t)\Phi_j(\boldsymbol{\xi})}$$

$(M+1) = (N+P)!/(N!P!)$

avec $\boldsymbol{\xi} = (\xi_1, \cdots, \xi_N)^T$ n'est **pas** limité à une distribution gaussienne!

N: dimension de l'espace probabiliste

P : ordre le plus élevé du polynôme

Moyenne: $\overline{X(\omega)} =< X(\omega) >= a_0$

Variance: $\mathrm{var}(X(\omega)) =< \left(X(\omega) - \overline{X(\omega)}\right)^2 >= \sum_{j=1}^{P} a_j^2 < \Phi_j^2 >$

Exemple:

- $\boldsymbol{\xi}$: distribution gaussienne
- Φ : Polynômes d'Hermite
- N=2; P=2

$$\begin{aligned}
\Phi_0(\boldsymbol{\xi}) &= 1.0\\
\Phi_1(\boldsymbol{\xi}) &= \xi_1\\
\Phi_2(\boldsymbol{\xi}) &= \xi_2\\
\Phi_3(\boldsymbol{\xi}) &= \xi_1^2 - 1\\
\Phi_4(\boldsymbol{\xi}) &= \xi_2^2 - 2\\
\Phi_5(\boldsymbol{\xi}) &= \xi_1\xi_2
\end{aligned}$$

Technique d'utilisation du PC pour la résolution d'équation différentielle stochastique

Approche *INTRUSIVE* (method of weighted residuals)

$$\boxed{\mathcal{L}(\mathbf{x}, t, \omega; u) = f(\mathbf{x}, t; \omega),} \qquad x \in D(\Lambda), t \in (0, T), \omega \in \Omega,$$

1/ Discrétiser le processus aléatoire à l'aide de variables aléatoires (indépendantes).

$$\boldsymbol{\xi}(\omega) = \{\xi_1(\omega), \cdot, \xi_N(\omega)\}$$

$$\mathcal{L}(\mathbf{x}, t, \boldsymbol{\xi}; u(x, t; \boldsymbol{\xi})) = f(\mathbf{x}, t; \boldsymbol{\xi})$$

2/ Ecrire la solution et les paramètres d'entrée incertains sous forme de sommes *finies* de PC et substituer dans l'équation.

$$\mathcal{L}\left(\mathbf{x}, t, \boldsymbol{\xi}(\omega); \sum_{i=0}^{M} u_i \Phi_i(\boldsymbol{\xi}(\omega)\right) = f(\mathbf{x}, t; \boldsymbol{\xi}(\omega))$$

3/ Projeter (type Galerkin) sur la base des polynômes orthogonaux considérés. Obtention d'un système linéaire.

$$\left\langle \mathcal{L}\left(\mathbf{x}, t, \boldsymbol{\xi}; \sum_{i=0}^{M} u_i \Phi_i(\boldsymbol{\xi})\right), \Phi_k(\boldsymbol{\xi}) \right\rangle = \langle f, \Phi_k(\boldsymbol{\xi}) \rangle, \qquad k = 0, 1, \cdots, M$$

- les modes PC sont couplés de façon implicite
- nécessite l'adaptation du solver déterministe

Technique d'utilisation du PC pour la résolution d'équation différentielle stochastique

Approche *NON-INTRUSIVE* (collocation method)

$$\boxed{\mathcal{L}(\mathbf{x}, t, \omega; u) = f(\mathbf{x}, t; \omega),} \qquad x \in D(\Lambda), t \in (0, T), \omega \in \Omega,$$

1/ Discrétiser le processus aléatoire à l'aide de variables aléatoires (indépendantes).

$$\boldsymbol{\xi}(\omega) = \{\xi_1(\omega), \cdot, \xi_N(\omega)\}$$

$$\mathcal{L}(\mathbf{x}, t, \boldsymbol{\xi}; u(x, t; \boldsymbol{\xi})) = f(\mathbf{x}, t; \boldsymbol{\xi})$$

2/ Obtenir les coefficients PC en projetant la solution sur la base polynomiale.

$$(\forall k \in \{0, \ldots, P\}) \quad u_k = \frac{< u(\omega) \; \Phi_k(\boldsymbol{\xi}(\omega)) >}{< \Phi_k^2(\boldsymbol{\xi}(\omega)) >}$$

Finalement on a: $$u = \sum_{i=0}^{M} u_i \Phi_i(\boldsymbol{\xi}(\omega)$$

- revient au calcul de nombreuses quadratures numériques
- risque *d'aliasing*
- simplicité d'utilisation ne nécessite pas l'adaptation du solver déterministe (boite noire)

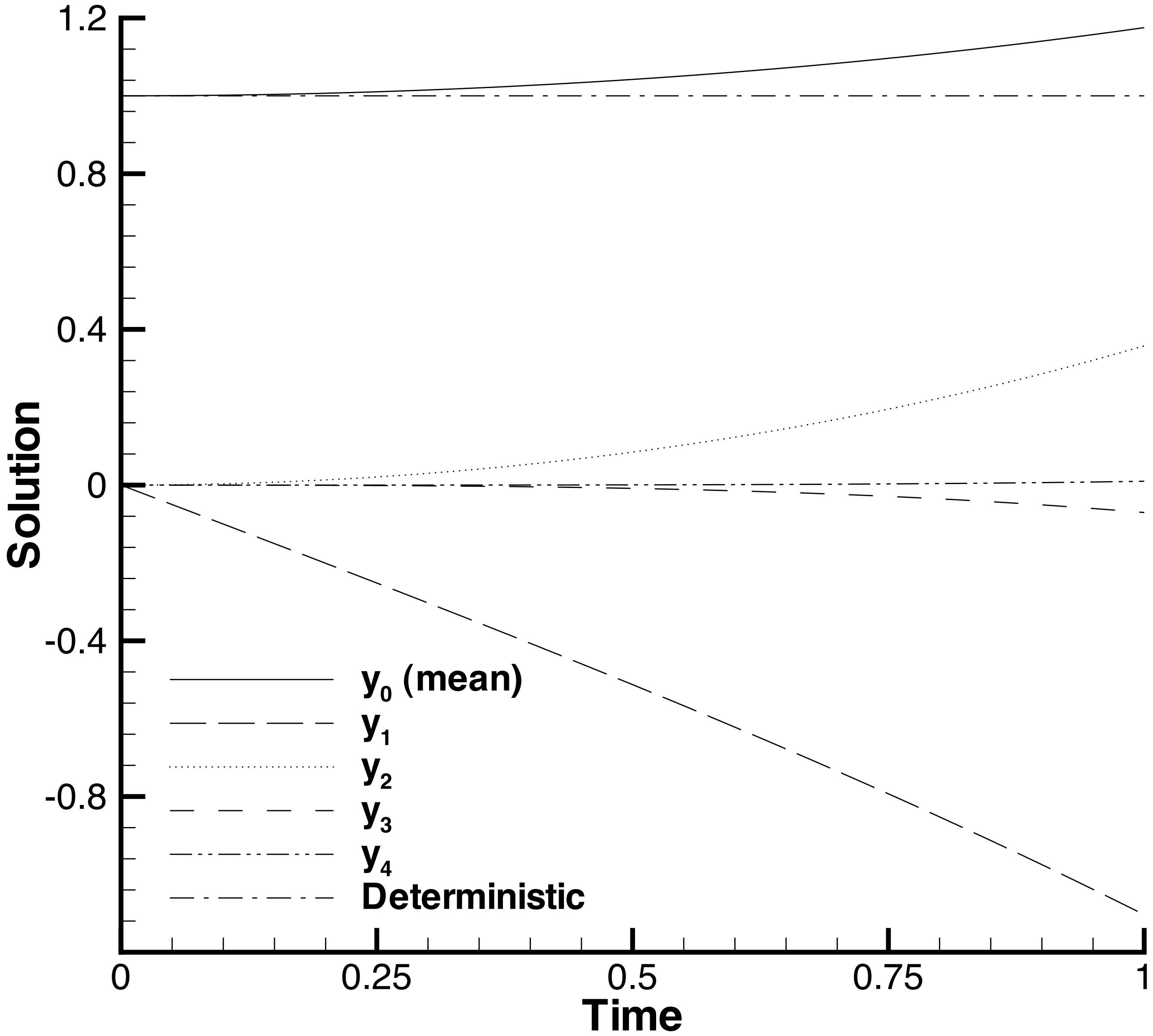
Example: 1st order linear ODE

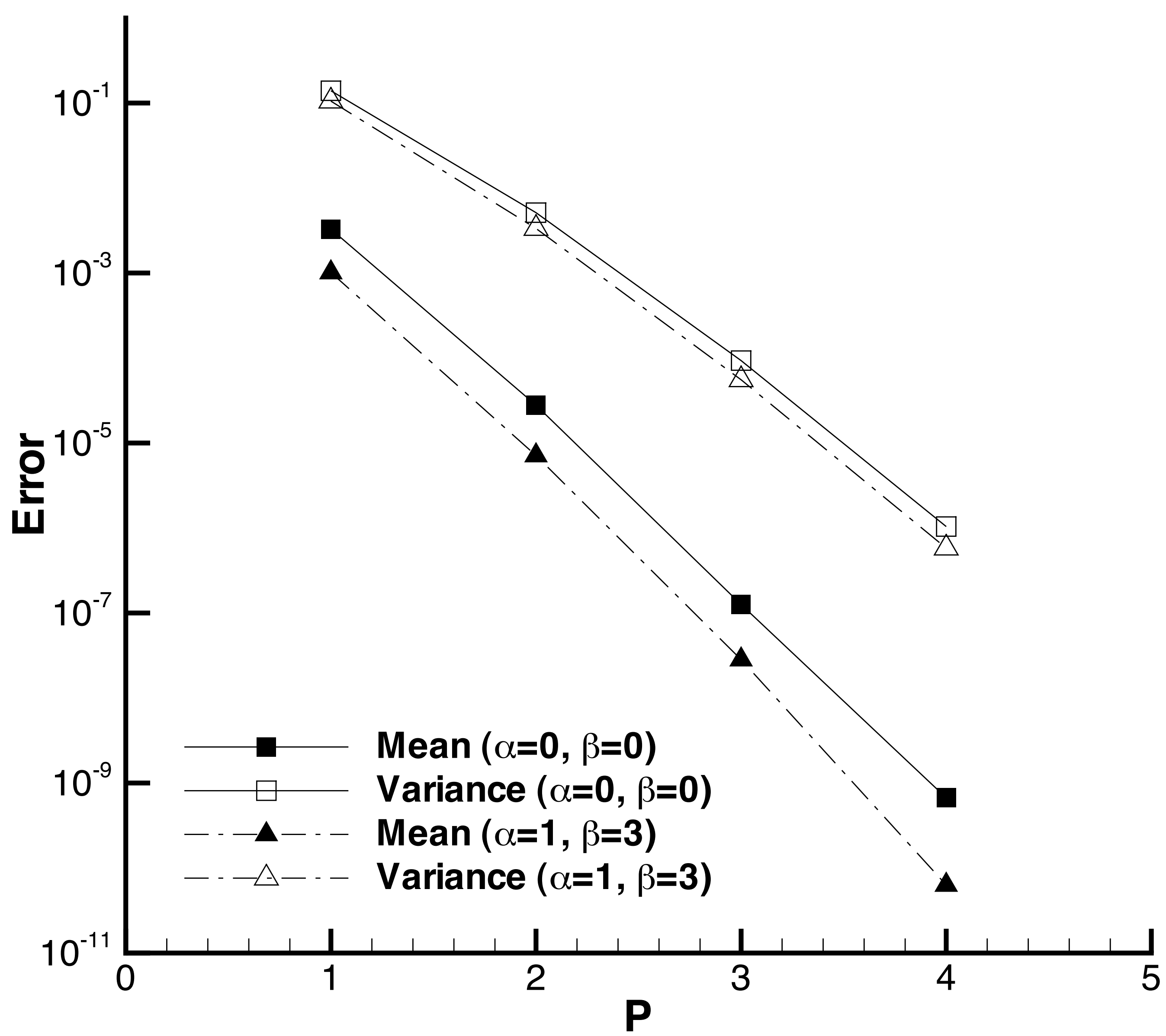
$$\frac{dy}{dt}(t,\omega) = -k(\omega)y, \qquad y(0) = \hat{y}, t \in (0,T) \qquad k = \bar{k} + \sigma_k \xi$$

$$y(t,\omega) = \hat{y}e^{-k(\omega)t} \qquad y(t,\omega) = \sum_{i=0}^{M} y_i(t)\Phi_i(\xi(\omega)), \qquad k(\omega) = \sum_{i=0}^{M} k_i \Phi_i(\xi(\omega)).$$

Galerkin projection: $$\frac{dy_l}{dt} = -\frac{1}{<\Phi_l^2>} \sum_{i=0}^{M} \sum_{j=0}^{M} <\Phi_i \Phi_j \Phi_l> k_i y_j \quad \text{for} \quad l = 0, 1, \ldots, M$$

$$f(k;\alpha,\beta) = \frac{(1-k)^\alpha (1+k)^\beta}{2^{\alpha+\beta+1} B(\alpha+1, \beta+1)}, \qquad -1 < k < 1, \ \alpha, \beta > -1$$





Avantages des méthodes gPC

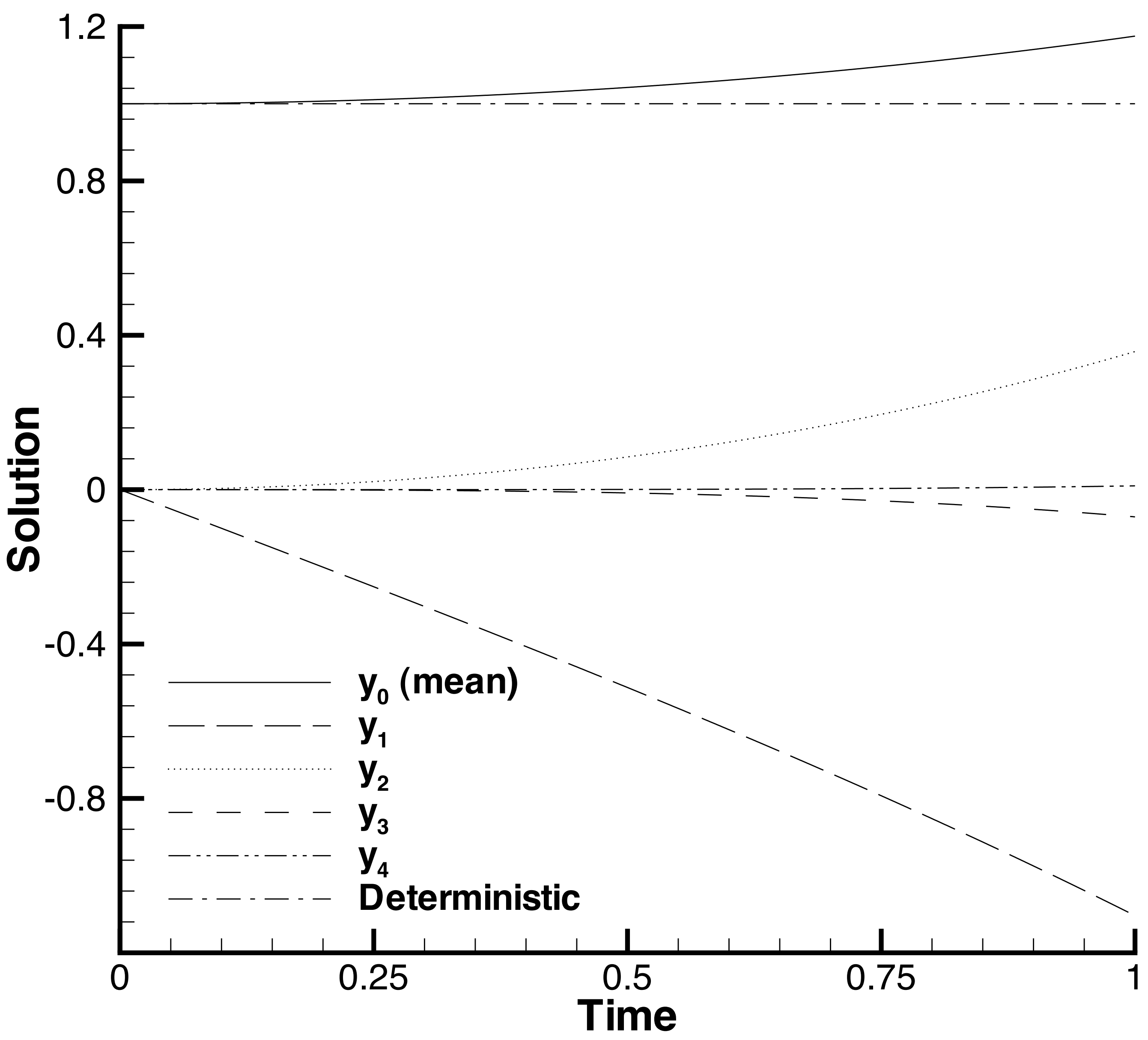
- Méthode efficace qui fournit une estimation quantitative de la sensibilité de la solution aux incertitudes des parametres d'entrée
- Convergence spectrale et représentation optimale (compacité et précision) de l'incertitude grâce à un choix de polynômes appropriés. Possibilité de représentation non-intrusive par projection de la solution sur la base du chaos polynomial.
- Non limitée aux distributions gaussiennes d'incertitude ou à des incertitudes faibles.
- Tous les moments + pdf de la solution sont disponibles.
- Coût de calcul en général très inférieur aux méthodes de type Monte-Carlo (distribution gaussienne: 1 à 2 ordres de grandeur, distribution uniforme: 3 à 4 ordres de grandeur).

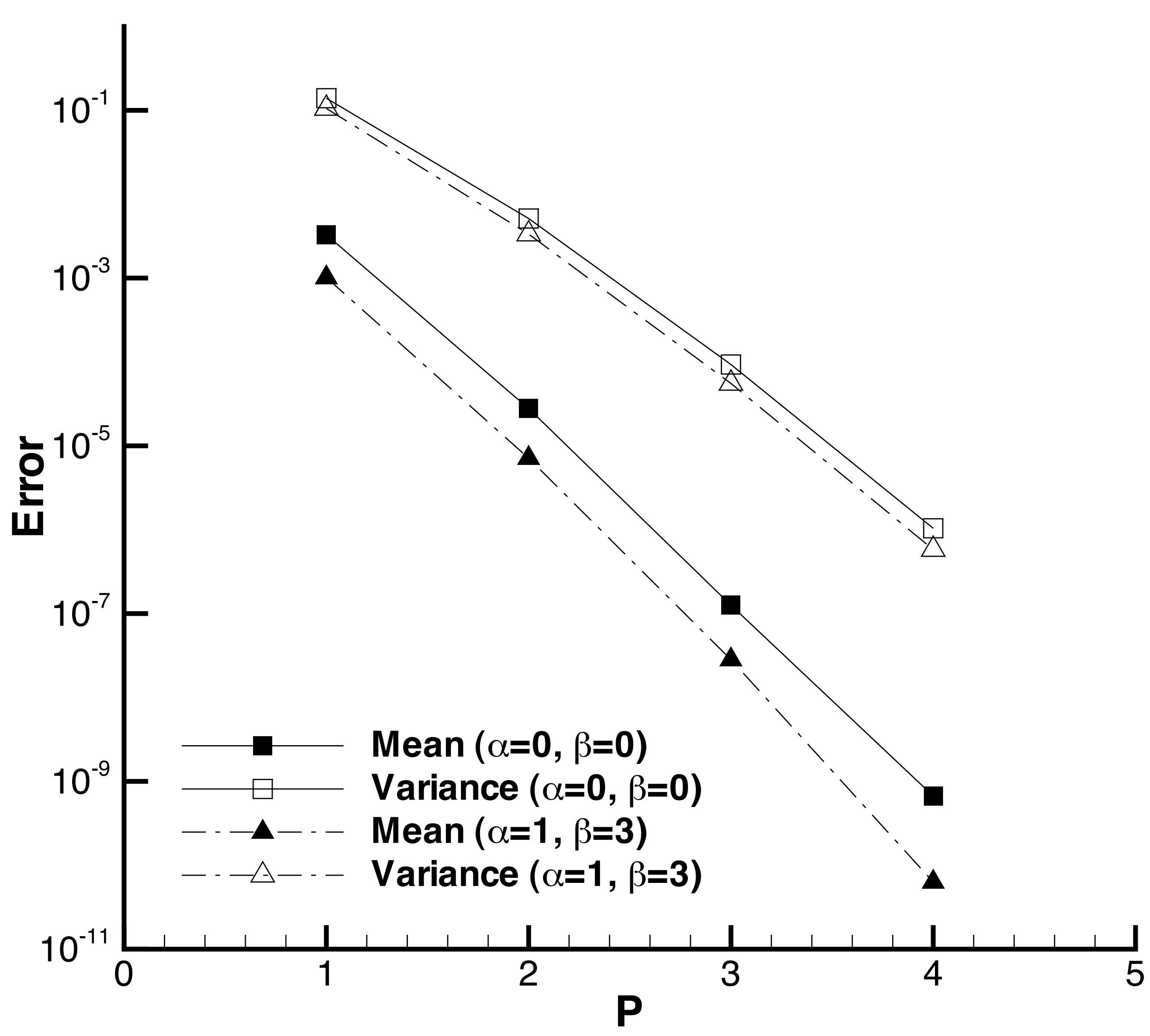
Difficulty of the method

$$\frac{dy}{dt}(t,\omega) = -k(\omega)y, \qquad y(0)=\hat{y}, t\in(0,T) \qquad k=\bar{k}+\sigma_k\xi$$

$$y(t,\omega)=\hat{y}e^{-k(\omega)t} \qquad y(t,\omega)=\sum_{i=0}^{M} y_i(t)\Phi_i(\xi(\omega)), \qquad k(\omega)=\sum_{i=0}^{M} k_i\Phi_i(\xi(\omega)).$$

$$f(k;\alpha,\beta)=\frac{(1-k)^\alpha(1+k)^\beta}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}, \qquad -1<k<1,\ \alpha,\beta>-1$$





Effect of GPC variable order P on the convergence rate in time

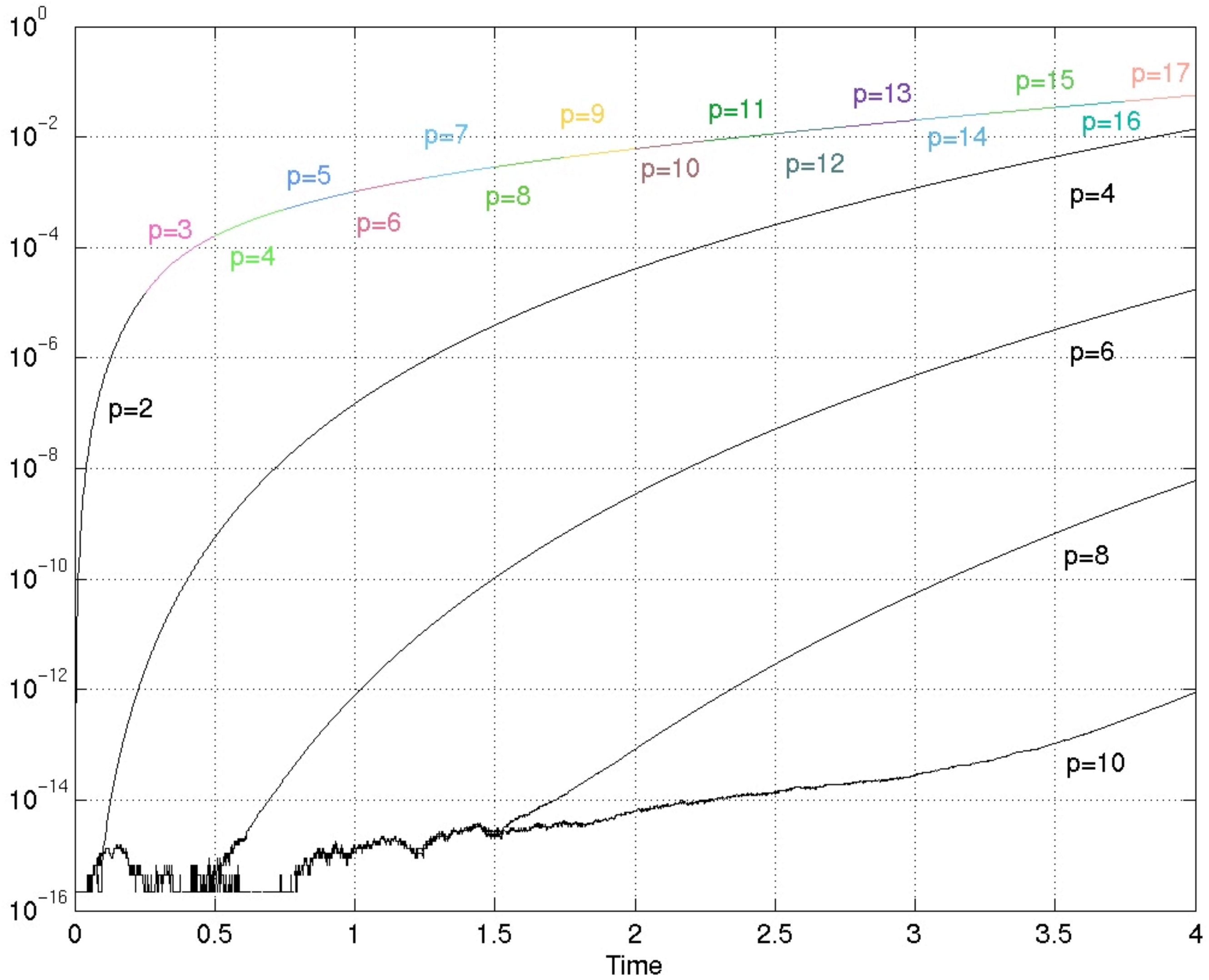
$$\begin{cases} \dfrac{dx}{dt} = -kx \quad t \in [0,T] \\ x(t=0) = x_0 \end{cases}$$

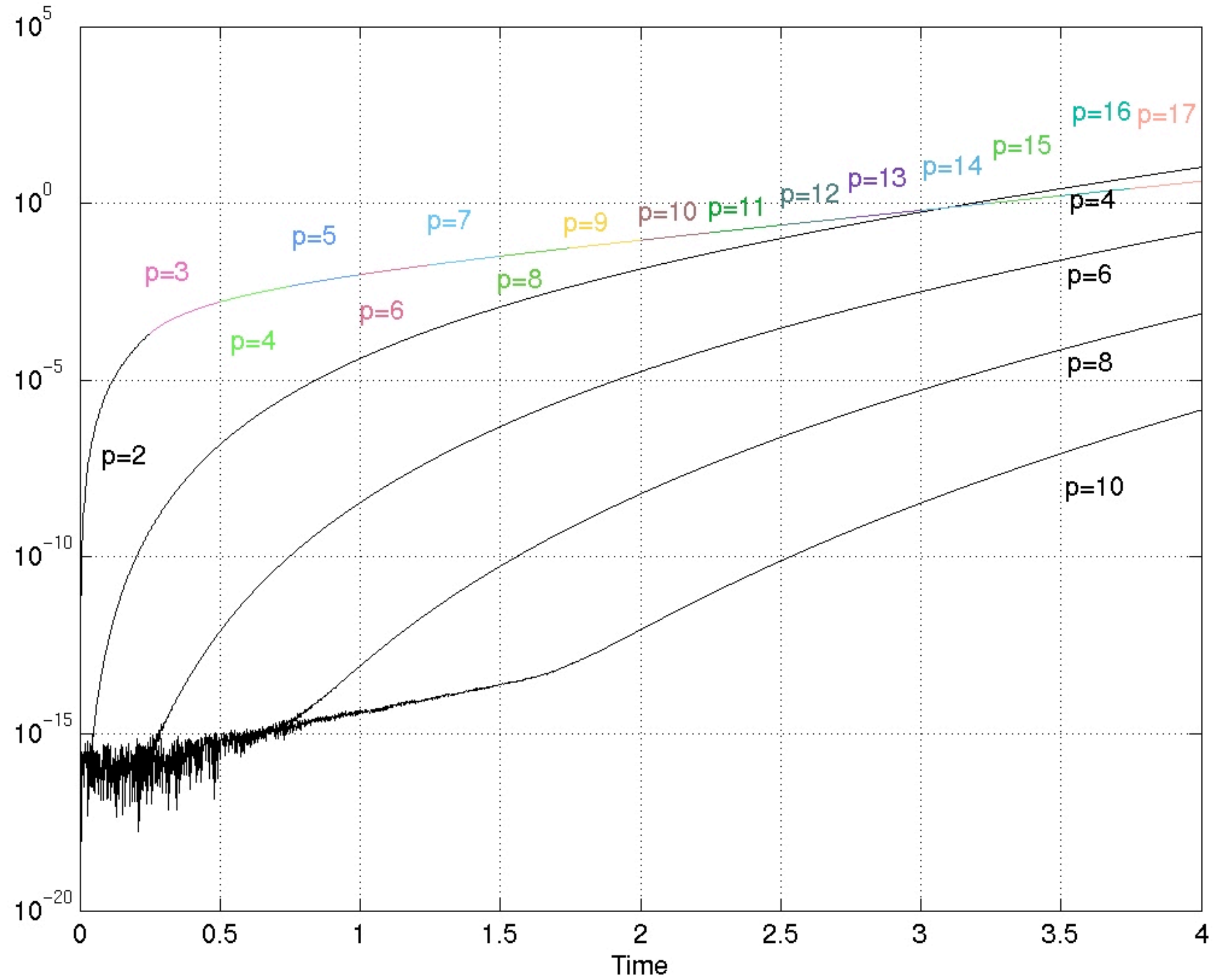
$$k = \bar{k} + \sigma\xi(\theta)$$

k is a *random variable* with zero mean and constant variance and a certain probability distribution f(k) : Uniform distribution (Legendre)

Mean solution: $\bar{x}(t) = \int_{\Omega} x_0 e^{-kt} f(k)\,dk$

Variance solution: $\langle x^2(t) \rangle = \int_{\Omega} \left(x_0 e^{-kt} - \bar{x}(t)\right)^2 f(k)\,dk$





Difficulty of the method

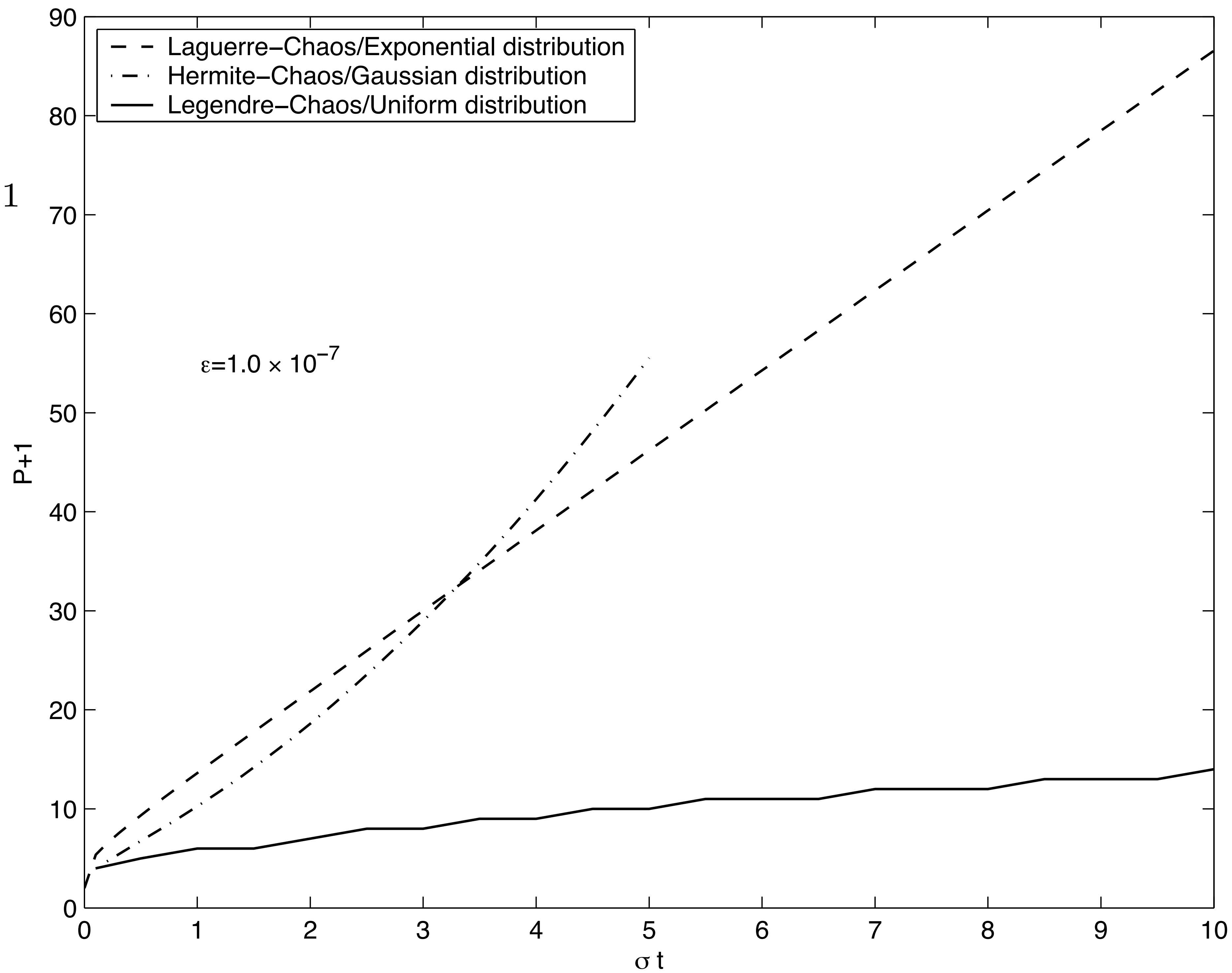
$$\epsilon_P = \langle (y(t) - y_P(t))^2 \rangle / \langle y^2(t) \rangle$$

Gaussian/Hermite

$$\epsilon_P \leq \frac{(\sigma t)^{2(P+1)}}{e^{(\sigma t)^2} - 1} \left[(P+1)! \left(1 - \frac{(\sigma t)^2}{P+1} \right) \right]^{-1}$$

Exponential/Laguerre

$$\epsilon_P = \left(\frac{\sigma t}{1 + \sigma t} \right)^{2P}$$



Problems and possible remedies...

- Spectral estimation of non-linear terms when no closed-forms are available
  - use pseudo-spectral approximation.
- Low convergence for non-Gaussian process:
  - use the appropriate measure with Generalized PC.
- Convergence failure for discontinuous or non-smooth processes (stochastic bifurcation)
  - develop adapted (non-smooth or local) bases: multi-wavelets or multi-elements gPC.
- CPU cost for large scale problems
  - design new solvers, use different types of (sparse) numerical quadratures, sparse tensor products.
- Challenge: development of bases and techniques to improve convergence and robustness of spectral expansions for processes with steep/discontinuous dependences to uncertain parameters or processes depending on a <u>large</u> number of random variables.

Possible applications so far...

- Solid mechanics (Ghanem & Spanos 1989-91).
- Flow through porous media (Ghanem & Dham 1998, Zhang & Lu 2004).
- Heat diffusion in stochastic media (Hien & Kleiber 1997-98, Xiu & Karniadakis 2003).
- Incompressible flows (Le Maître et al, Karniadakis et al, Hou et al).
- Fluid-Structure interaction (Karniadakis et al).
- Micro-fluid systems (Debusschere et al 2001).
- Reacting flows & combustion (Reagan et al 2001).
- 0-Mach flows & thermo-fluid problems (Le Maître et al 2003).