Spectral approach to UQ

- Probabilistic approach to UQ

- Stochastic solution is sought in a product space
  - probability space (x axis)
  - deterministic solution space (y axis)
  - both are assumed to have Hilbert space structure, with a countable orthogonal basis
Spectral Expansion

- mean-square convergent expansion in the space of random variables:

\[ u(x, t; \xi) = \sum_{k} u_k(x, t) \Psi_k(\xi) \]

- solution mode
- vector of canonical random variables that are suitably used to parametrize the uncertain inputs
- orthogonal basis in the space of square integrable random functions
- solution mode (coordinate in Hilbert space) is unknown to be determined
Examples

- **Legendre:**
  \[ Le_n(x) = \frac{1}{2^n} \sum_{l=0}^{[n/2]} (-1)^l \binom{n}{l} \binom{2n - 2l}{n} x^{n-2l} \]

  - orthogonal over \([-1,1]\) with uniform measure

- **Hermite:**
  \[ He_n(x) = n! \sum_{m=0}^{[n/2]} (-1)^m \frac{1}{m!2^m(n-2m)!} x^{n-2m} \]

  - orthogonal over \((-\infty,\infty)\) with Gaussian measure
Determination of coefficients

- **Intrusive approach:**
  - Generally Galerkin formalism – insert expansion into governing equations and derive governing equations for coefficients

- **Non-intrusive approach:**
  - Reconstruct functional relation based on discrete realizations
  - Regression approaches (including Bayesian regression)
  - Spectral projection (Gauss quadratures, sparse quadratures, adaptive quadratures, MC quadratures, ...)
  - Compressing sensing (CS, BCS)
  - Etc...
Why spectral expansions?

- Efficiency:
  - provided, generally, that sufficient smoothness is present

- Probabilistic framework:
  - provides fundamental tools for analyzing stochastic errors, convergence, etc...

- Format:
  - key to the machinery of approximation theory
    (optimization, sensitivity analysis, inverse design, etc...)
Non-Intrusive Spectral Projection (NISP)

- Alternative to Galerkin formalism in situations where modification of production or legacy codes is not feasible
- Essentially a collocation approach to the evaluation of probability integrals

\[
\langle \Psi_k^2 \rangle Q_k = \langle Q(\xi) \Psi_k(\xi) \rangle \approx \sum_{i=1}^{N} Q(x_i) w_i
\]

uncertain inputs $\rightarrow$ Model $\rightarrow$ quantity of interest
Sparse quadratures

- **Smolyak/Gauss Patterson**
  - non-adaptive
  - nested grid
  - level $p$ resolution $\sim$ yields order $p$ PC

- **Adaptive extension**
  - variance-based error indicators
  - “optimal” pseudo-spectral construction

- Both approaches well suited to moderate dimensionality
Smolyak pseudospectral construction

- New Smolyak pseudospectral approximation (Constantine et al., 2011; Conrad & Marzouk, 2012):
  - essentially a telescoping sum of pseudospectral projections (each internal-aliasing-free)
  - enables inclusion of all polynomials on general sparse grid that can be computed without internal aliasing
  - efficient use of data
  - adaptive variants avoid hand tuning
UQ Toolkit

- **UQ Toolkit** provides library of subroutines that implement moment formulas, approximate evaluations of various nonlinear transformations, post-processing functionals.

*Take-away:* essential comfort in the machinery that transform $f(u)$ into $[f(u)]_k$, without explicit need to manipulate moment expressions, yet keeping error control in mind.

- UQ Toolkit available as open source software at:
  
  [http://www.sandia.gov/UQToolkit/]