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Application of the Generalised Polynomial Chaos method to the transport equation

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Sensitivity Methods: Overview

- Estimates the effect of numerous perturbations on reactor parameters.
- Neglects change in flux due to perturbations. Corrected with GPT and variational methods.
- Wide application throughout reactor analysis.

Sensitivity Methods: Diffusion Example

The perturbed and unperturbed diffusion operators

$$L = \frac{d^2}{dx^2} D + \lambda \Sigma_f - \Sigma_a$$
$$L' = \frac{d^2}{dx^2} D' + \lambda' \Sigma_f' - \Sigma_a'$$

where

$$D' = D + \Delta D$$
$$\Sigma' = \Sigma + \Delta \Sigma$$
$$\lambda' = \lambda + \Delta \lambda$$

Sensitivity Methods: Diffusion Example

The fundamental result from first order perturbation theory

$$(\phi^\dagger, \delta L \phi') = 0$$

where $\phi^\dagger$ is the adjoint flux, ϕ' is the perturbed flux and

$$\delta L = L' - L$$

we may write the change in the eigenvalue

$$\Delta\lambda = -\frac{(\phi^\dagger, \Delta D \frac{d^2\phi}{dx^2}) + \lambda(\phi^\dagger, \Delta\Sigma_f \phi) - (\phi^\dagger, \Delta\Sigma_a \phi)}{(\phi^\dagger, \Delta\Sigma_f \phi) + (\phi^\dagger, \Sigma_f \phi)}$$

Spectral Expansion Methods: Overview

- Introduce uncertainty explicitly into the governing equations
- Paramerterise inputs in terms of a set of independant random variables $\xi = (\xi_1, \xi_2, \cdots, \xi_M)$ and project on to a stochastic space.
- The output/input of the model is expressed in a fourier like expansion:

$$r(x,t,\xi) = \sum_{i=0}^{\infty} r_i(x,t)\psi_i(\xi)$$

Karhunun Loeve (KL) Expansion

- Discretise a spatially varying random process in terms of the eigenvalues and eigenvectors of its covariance function.
- Truncate expansion at some value d. d is inversly proportional to the correlation length.
- Optimal in the mean square sense when truncating after d terms.

$$\Sigma(x,\omega) = <\Sigma(x)> + \sum_{k=1}^{\infty} \sqrt{\lambda_k}\varphi_k(x)\xi(\omega)$$

$$\int_X C_\Sigma(x_1,x_2)\varphi_k(x_2)dx_2 = \lambda_k\varphi_k(x_1)$$

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Karhunun Loeve (KL) Expansion

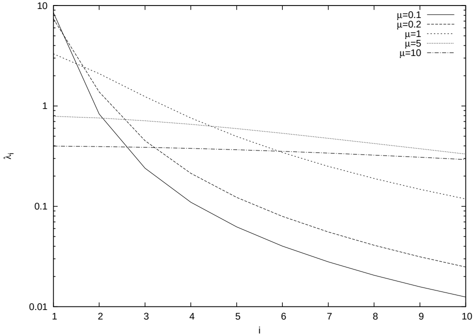

Figure: Eigenvalues for the exponential covariance function at different correlation lengths (b=5.0, $\sigma_{\Sigma}^2 = 2.0$).

Generalised Polynomial Chaos

- Generalization of homogenous chaos.
- Convergence of homogenous chaos is dependant on the distribution of the random variables.
- GPC outlines which polynomial basis is optimal for the type of random variable.

Wiener-Askey Chaos	Random Variables	Support
Hermite	Gaussian	$(-\infty, \infty)$
Laguerre	gamma	$[0, \infty)$
Jacobi	beta	$[a, b]$
Legendre	uniform	$[a, b]$

Generalised Polynomial Chaos

The output stochastic process $U(x, \xi)$ can be expressed by the expansion:

$$U(x, \xi) = \sum_{i=0}^{N_P} U_i(x)\Phi_i(\xi) \tag{1}$$

The first two moments of the output process are:

$$\begin{aligned} \bar{U} &= E[U] = U_0 \\ \sigma_U &= E[(N - E[U])^2] \\ &= \sum_{i=1}^{N_p} U_i^2 \left\langle \Phi_i^2(\xi) \right\rangle \end{aligned} \tag{2}$$

Generalised Polynomial Chaos - SMoC

The one dimensional forward characteristic form of the stochastic neutron transport equation:

$$\frac{d\phi(x+s\mu,\mu,\xi)}{ds}+\Sigma_t(x+s\mu,\xi)\phi(x+s\mu,\mu,\xi)=q(x+s\mu,\xi) \tag{3}$$

- $q(x+s\mu,\xi)$ is the sum of the scattering, fission and extraneous sources.
- Σ_t and Σ_{S_0} are the transport and isotropic scattering cross sections.
- $\phi(x+s\mu,\mu,\xi)$ is the uncertain angular flux.

Generalised Polynomial Chaos - SMoC

Expand the angular flux using a PCE of the form

$$\phi(x + s\mu_m, \mu_m, \xi) = \sum_{i=0}^{N_P} \phi_i(x + s\mu_m, \mu_m)\Phi_i(\xi) \tag{4}$$

Projecting on to the basis Φ_j and taking the mathematical expectation yields

$$\frac{d\hat{\phi}(x + s\mu_m, \mu_m)}{ds} + A\hat{\phi}(x + s\mu_m, \mu_m)$$
$$= B \sum_{m=1}^{N_{quad}} \hat{\phi}(x + s\mu_m, \mu_m) w_m + < \Phi(\xi)\bar{q}^{ext} > \tag{5}$$

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Generalised Polynomial Chaos - SMoC

Matrices A and B are symmetric

$$A_{ji}(\xi) = \frac{< \Phi_j(\xi)\Sigma_t(\xi)\Phi_i(\xi) >}{N_i N_j} \quad ; \quad B_{ji}(\xi) \quad = \frac{< \Phi_j(\xi)\Sigma_{S0}(\xi)\Phi_i(\xi) >}{N_i N_j}$$

Diagonalising the matrix A gives

$$\frac{d\psi_j(x+s\mu_m,\mu_m)}{ds} + \Lambda_j\psi_j(x+s\mu_m,\mu_m)$$
$$= \sum_{i=0}^{N_P} L^{-1}B_{ji}L\sum_{m=1}^{N_{quad}} \psi_i(x+s\mu_m,\mu_m)w_m + \Gamma_j \quad \forall j \qquad (6)$$

Generalised Polynomial Chaos - SMoC

$$\psi_i(S_{out}, \mu_m) = \psi_i(S_{in}, \mu_m)exp(-\Lambda_i \Delta S_m) + \frac{\bar{\Gamma}_i}{\Lambda_i}(1 - exp(-\Lambda_i \Delta S_m))) \quad (7)$$

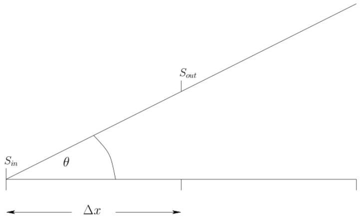

Figure: Cartesian space-angle coordinate system in one dimension.

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SMoC: Data for Numerical Results

Data for the one region problem

Region	Domain	Distribution	$\Sigma_{t\ min}$	$\Sigma_{t\ max}$	$\Sigma_{S\ min}$	$\Sigma_{S\ max}$	q^{ext}
1	[0:3.0]	Uniform	0.75	2.25	0.25	0.75	1.0

Data for the two correlated regions

Region	Domain	Distribution	$\Sigma_{t\ min}$	$\Sigma_{t\ max}$	$\Sigma_{S\ min}$	$\Sigma_{S\ max}$	q^{ext}
1	[0:1.5]	Uniform	0.75	2.25	0.25	0.75	1.0
2	[1.5:3.0]	Log-Uniform	1.25	3.75	0.40	1.20	1.0

Data for the two uncorrelated regions

Region	Domain	Distribution	$\Sigma_{t\ min}$	$\Sigma_{t\ max}$	$\Sigma_{S\ min}$	$\Sigma_{S\ max}$	q^{ext}
1	[0:1.5]	Uniform	0.75	2.25	0.25	0.75	1.0
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SMoC: One Region Problem

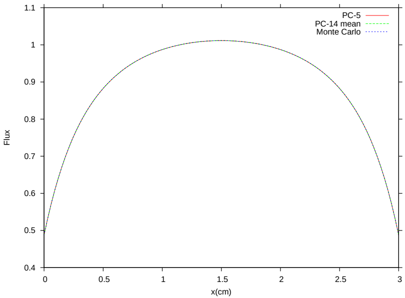

Figure: Mean in the scalar flux for the one region SMoC Problem.

SMoC: One Region Problem

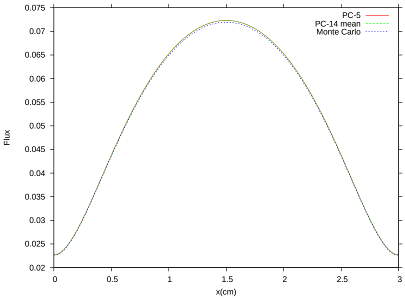

Figure: Variance in the scalar flux for the one region SMoC Problem.

SMoC: One Region Problem

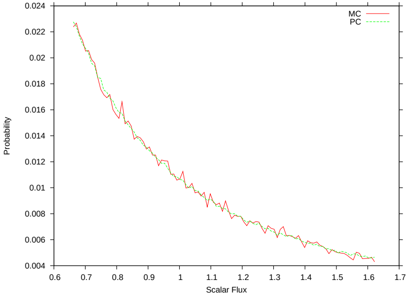

Figure: Probability density function of the scalar flux for the one region problem at $x = 1.5$ cm.

SMoC: Two Correlated Regions

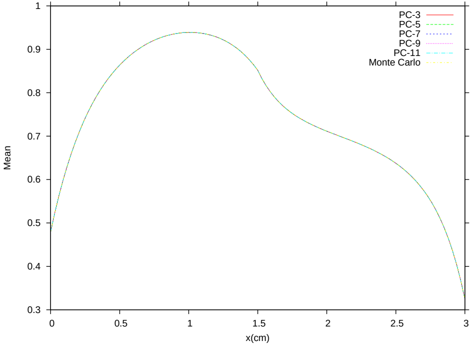

Figure: Mean in the scalar flux for the two region SMoC Problem.

SMoC: Two Correlated Regions

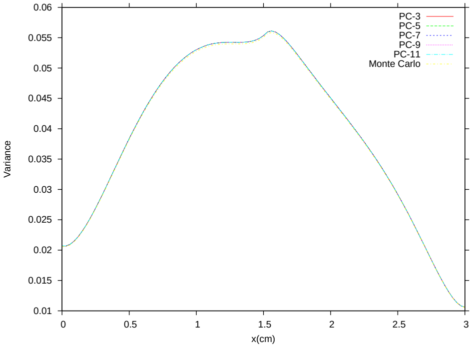

Figure: Mean in the scalar flux for the two region SMoC Problem.

SMoC: Two Correlated Regions

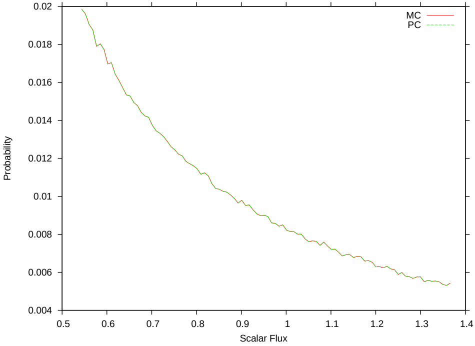

Figure: Probability density function of the scalar flux for the two correlated region problem at $x = 1.5$ cm.

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SMoC: Two Un-Correlated Regions

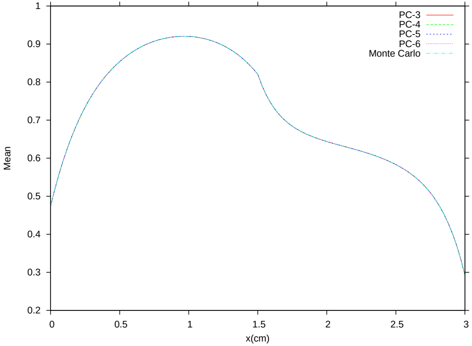

Figure: Mean in the scalar flux for the two un-correlated region problem.

SMoC: Two Un-Correlated Regions

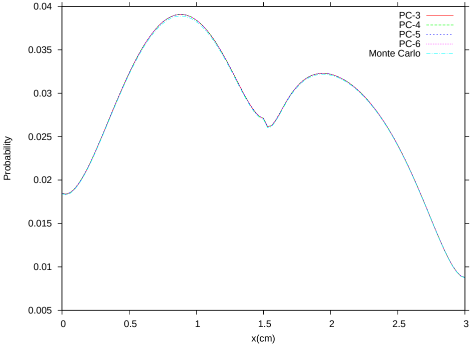

Figure: Variance in the scalar flux for the two un-correlated region problem.

SMoC: Two Un-Correlated Regions

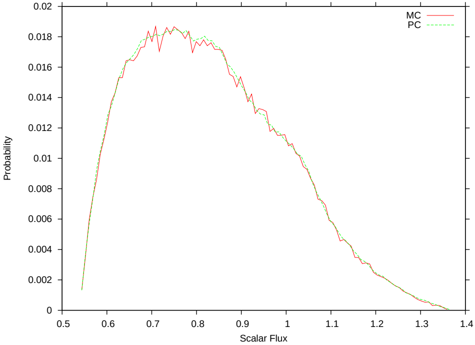

Figure: Probability density function of the scalar flux for the two un-correlated region problem at $x = 1.5$ cm.

Stochastic Finite Elements

First, the spatial domain is discretised using the normal FE method

$$U^{\dagger}(x,\xi) = \sum_{i=1}^{N_e} U_i(\xi) N_i(x) \tag{8}$$

Next, the parameters $U_i(\xi)$ are expanded in a PCE to give

$$U^{\dagger}(x,\xi) = \sum_{i=1}^{N_e} \left(\sum_{p=0}^{N_p} U_{ip} \Phi_p(\xi) \right) N_i(x)$$

SFEM: Diffusion with K_{eff} Uncertainty

K_{eff} is an output stochastic process so we expand in terms of a PCE

$$\lambda(\xi) = \frac{1}{K_{eff}(\xi)} = \sum_{k=0}^{N_p} \lambda_k \Phi_k(\xi)$$

The final equation set is

$$\sum_{i=0}^{N_p} \mathbf{K} e_{ji}\phi_j + \mathbf{M}(\Sigma_{t_0} - \Sigma_S)\phi_j + \mathbf{M} f_{ji}\phi_j = \sum_{i=0}^{N_p}\sum_{k=0}^{N_p} \mathbf{M}\nu\Sigma_f \phi_j \lambda_k C_{jki}$$

SFEM: Diffusion with K_{eff} Uncertainty

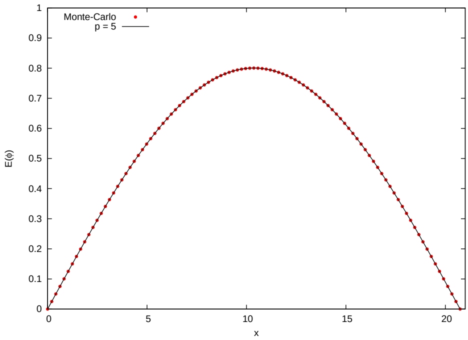

Figure: Mean in the scalar flux for the stochastic diffusion problem.

SFEM: Diffusion with K_{eff} Uncertainty

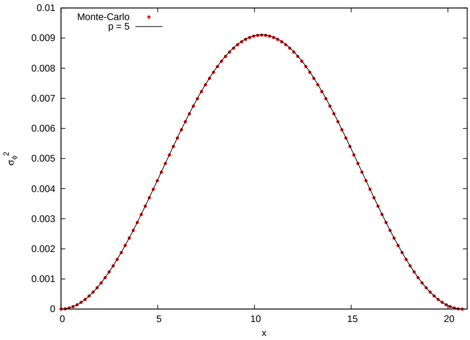

Figure: Variance in the scalar flux for the stochastic diffusion problem.

SFEM: Diffusion with K_{eff} Uncertainty

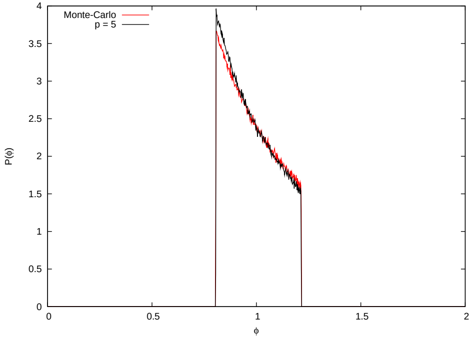

Figure: Probability density function of K_{eff} for the stochastic diffusion problem.

Future Work

- Stochastic transport and sensitivity methods in 2 and 3 dimensions for fixed source and multiplying systems (Diffusion, LD-SN, LD-PN, MOC).
- Spatial and point kinetics models.
- Burnup.
- Adaptive SFEM already developed by Andrew Hagues for time dependant non-linear problems using goal based error measures (as per Mark Goffin's talk).
- AMCG will integrate discretisation error (Mark Goffin's work), my uncertainty work and James Dyrda's work on data assimilation to obtain a measure of the total error in neutron transport calculations.

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