Introduction to Uncertainty Quantification
Module 3: Uncertainty Propagation

Often in uncertainty quantification, our objective is to understand the influence of uncertainty in the input of a system on the output, or response of the system. This problem is referred to as *uncertainty propagation* because we aim to propagate the uncertainty through the equations that govern the system. When uncertainty in the input is specified probabilistically, as we will consider here, the problem can be posed mathematically as follows.

Given a random vector, $\boldsymbol{X}$, having joint PDF $f_{\boldsymbol{X}}(\boldsymbol{x})$ (joint CDF $F_{\boldsymbol{X}}(\boldsymbol{x})$), we consider the general operator $\boldsymbol{Y} = G(\boldsymbol{X})$ that takes $\boldsymbol{X}$ as input and produces the random vector $\boldsymbol{Y}$. In it's most complete formulation, the goal of uncertainty propagation is to determine the joint PDF of $\boldsymbol{Y}$, $f_{\boldsymbol{Y}}(\boldsymbol{y})$ or equivalently the joint CDF $F_{\boldsymbol{Y}}(\boldsymbol{y})$. In many cases, discovering the complete PDF or CDF of $\boldsymbol{Y}$ exactly (i.e. analytically) is impossible – especially if the operator $G(\cdot)$ is very complex (have many degrees of freedom, nonlinear or non-smooth behavior) and/or when $\boldsymbol{X}$ and $\boldsymbol{Y}$ are high-dimensional. In these cases, we aim to develop methods to approximate the distribution of $\boldsymbol{Y}$ (or the marginal distributions of certain important components) or estimates the properties (i.e. moments) of the distribution.

Many approaches have been developed to estimate uncertainty in the response of mathematical / physical systems with uncertain input. In this module, we will introduce several of the most commonly used approaches for uncertainty propagation. We will start with methods that are capable of treating relatively simple systems analytically and will build in complexity. In particular, we will explore the following approaches:

- *Functions of Random Variables:* First, we will see how uncertainty can be propagated through relatively simple functions of random variables using the *Change of Variables Theorem.* We will see that this works very nicely for simple functions, but becomes very complicated for systems that are not uniquely invertible and continuous.

- *Expansion / Perturbation Methods:* Here, we will see how approximating the system through a Taylor series expansion allows us to estimate the moments of the system. We will see that these moment estimates are exact when the system depends linearly on the random variables $\boldsymbol{X}$ and that these so-called perturbation methods can be accurate for mildly nonlinear systems.

- *Monte Carlo Simulation:* We with then introduce the most commonly used and most robust method for uncertainty propagation, the Monte Carlo method. We will see that the Monte Carlo method relies on statistical estimates of the properties of $\boldsymbol{Y}$ from randomly generated realizations of the input $\boldsymbol{X}$, and while it is robust to system complexity (it can handle strongly nonlinear and discontinuous operations) and dimension (convergence does not depend on problem dimension) it is slow to converge. We therefore provide a brief introduction to the class of *variance reduction* techniques that aim to improve its efficiency.

- *Surrogate Models:* A common approach in uncertainty propagation is to develop an inexpensive function $\tilde{g}(\boldsymbol{X})$ that aims to approximate the operation $\boldsymbol{Y} = G(\boldsymbol{X})$. These models – often referred to as surrogate models, metamodels, or emulators – are then used to enable Monte Carlo simulations by making

approximate evaluation of the system computationally tractable. We will specifically introduce the two most commonly used surrogate models, polynomial chaos expansions and Gaussian process regression.

- *Numerical Methods:* Finally, we will conclude by introducing some more advanced numerical methods for the propagation of uncertainty – the stochastic spectral methods and stochastic collocation.