Uncertainty Quantification in Multiscale Computational Simulations of Dynamical Systems

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Uncertainties need to be taken into account for credible predictions of the response of complex mechanical systems. Such uncertainties should include uncertainties in the system parameters and those arising due to the modelling of a complex system. In spite of extensive research over the past four decades a general purpose probabilistic predictive code for real-life mechanical systems is still not available. The reasons behind this include: (a) the computational time can be prohibitively high compared to a deterministic analysis, and (b) the detailed and complete information regarding parametric and model uncertainties are in general not available. In this work various methods are investigated to address these two problems in the context of computational mechanics. The proposed methods can be broadly categorised as (a) parametric methods and (b) non-parametric methods. Under the parametric approaches, we have developed (1) high dimensional model representation (HDMR) method, and (2) Gaussian Process (GP) emulator approach. Under the nonparametric approaches we have developed a random matrix based approach. Several numerical and analytical techniques have been proposed and the results were validated against experimental results. As an application sensitivity and calibration of carbon nanotube base bio-sensors have been discussed. This poster is aimed at summarise these works and present some representative results.

Uncertainty quantification using Gaussian process emulators

A computer code implementation of a mathematical model, also known as *simulator*, can be understood as a function $\eta : \Omega \rightarrow \mathbb{R}^d$ whose domain is the p-dimensional parameter space $\Omega = \Omega_1 \times \ldots \times \Omega_p$. If a simulator is computationally intensive, a surrogate model can be employed to approximate its output. One such surrogate modeling strategy, known as *Gaussian process emulation*, makes it is possible to obtain a statistical approximation to the output of the simulator after evaluating only a small number of design points $\{\mathbf{x}_i\}_{i=1}^n \subseteq \Omega$. A Gaussian process emulator should satisfy some minimal criteria:

1. Since by definition the output at each design point is known, the emulator should reproduce this output with no uncertainty.
2. At any $\mathbf{x}$ that is not a design point, the probability distribution provided by the emulator should produce a mean value that constitutes a plausible interpolation of the training data. The probability distribution around this predictive mean should also express the uncertainty about how the emulator might interpolate.

Emulation works by generating a set of training runs $\mathbf{y} = \{\mathbf{x}_i, \eta(\mathbf{x}_i)\}_{i=1}^n$ that are treated as data used to update some prior beliefs about the simulator's output. These beliefs are represented by a Gaussian stochastic process prior distribution of the form

$$\eta(\cdot) \sim \mathcal{N}(m(\cdot), V(\cdot,\cdot)) \tag{1}$$

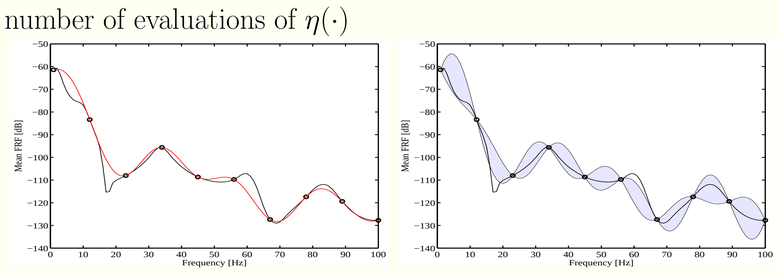
with $V(\mathbf{x}, \mathbf{x}') = \sigma^2 C(\mathbf{x}, \mathbf{x}')$, where

$$C(\mathbf{x}, \mathbf{x}') = e^{-(\mathbf{x}-\mathbf{x}')^{\mathrm{T}}\mathbf{B}(\mathbf{x}-\mathbf{x}')} \tag{2}$$

and σ^2 estimated from the data. $\mathbf{B}$ is a positive-definite diagonal matrix containing smoothness parameters that can be estimated using a maximum likelihood scheme.
Adopting the Bayesian paradigm, this prior distribution is updated with the objective information contained in the training runs $\mathbf{y}$, resulting in the posterior distribution

$$\eta(\cdot)|\mathbf{y} \sim \mathcal{N}(m^*(\cdot), V^*(\cdot,\cdot)) \tag{3}$$

The posterior mean $m^*(\cdot)$ approximates the output of the simulator at any untried $\mathbf{x} \in \Omega$, whereas it reproduces the known output at each design point. Additionally, the posterior variance $V^*(\cdot,\cdot)$ quantifies the uncertainty that arises from having only a limited number of evaluations of $\eta(\cdot)$



(a) Predictive mean of the emulator (b) Uncertainty bounds for the predictive mean

Emulation of the mean frequency response of a plate with random Young's modulus (in black). The posterior mean of the emulator (in red) interpolates the training runs (circles) and predicts the output at untried inputs. Simultaneously, the posterior variance provides uncertainty bounds (in gray) for such prediction. Note how the uncertainty is equal to zero in each one of the training runs.

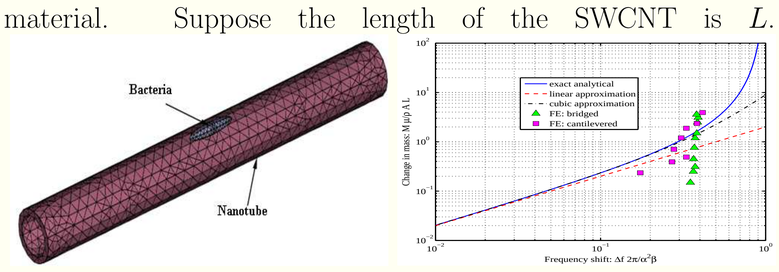
Carbon nanotube based bio-sensor

The potential of single-walled carbon nanotubes (SWCNTs) as a mass sensor is examined using continuum mechanics based approach. The carbon nanotube resonators are assumed to be either in cantilevered or in bridged configurations. Simple analytical formulas are developed for CNT-based nanoresonators with attached mass. A closed-form expression has been derived to detect the mass of biological objects from the frequency-shift. A simple linear approximation of the nonlinear sensor equation has been investigated. The validity and the accuracy of these formulas are examined for a wide range of cases.

In order to obtain simple analytical expressions of the mass of attached biochemical entities, we model a single walled CNT using a rod based on the Euler-Bernoulli beam theory. The equation of motion of free-vibration can be expressed as

$$EI\frac{\partial^2 y}{\partial x^2} + \rho A \frac{\partial^2 y}{\partial t^2} = 0 \tag{4}$$

where E the Youngs modulus, I the second moment of the cross-sectional area A, and ρ is the density of the material. Suppose the length of the SWCNT is L.



The general relationship between the normalized frequency-shift and normalized added mass of the bio-particles in a SWCNT with effective density ρ, cross-section area A and length L. Here $\beta = \sqrt{\frac{EI}{\rho A L^4}}\mathrm{s}^{-1}$, the nondimensional constant α depends on the boundary conditions and μ depends on the location of the mass. For a cantilevered SWCNT with a tip mass $\alpha^2 = \sqrt{140/11}$, $\mu = 140/33$ and for a bridged SWCNT with a mass at the midpoint $\alpha^2 = \sqrt{6720/13}$, $\mu = 35/13$. Relationship between the frequency-shift and added mass of bio-particles obtained from finite element simulation are also presented here to visualize the effectiveness of analytical formulas.
The numerical results indicate that the mass sensitivity of carbon nanotube-based nanobalances can reach upto 10^{-24} kg.

Random Matrix Theory for complex dynamical systems

The equation of motion of a damped n-degree-of-freedom linear dynamic system can be expressed as

$$\mathbf{M}\ddot{\mathbf{q}}(t) + \mathbf{C}\dot{\mathbf{q}}(t) + \mathbf{K}\mathbf{q}(t) = \mathbf{f}(t) \tag{5}$$

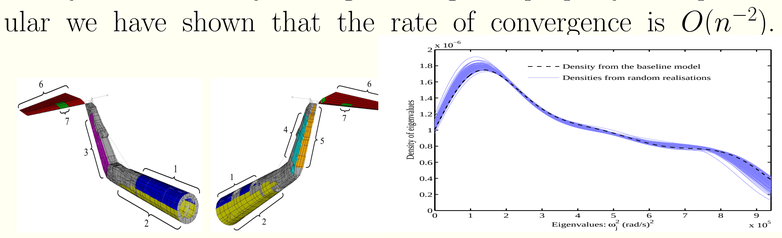
where $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$ are the mass, damping and stiffness matrices respectively. In order to completely quantify the uncertainties associated with system (5), we need the probability density functions of the random matrices $\mathbf{M}$, $\mathbf{C}$ and $\mathbf{K}$. These matrices can be expressed as Wishart matrices:
Wishart matrix: An $n \times n$ random symmetric positive definite matrix $\mathbf{S}$ is said to have a Wishart distribution with parameters $p \geq n$ and $\mathbf{\Sigma} \in \mathbb{R}_n^+$, if its pdf is given by

$$p_{\mathbf{S}}(\mathbf{S}) = \left\{2^{\frac{1}{2}np}\,\Gamma_n\left(\frac{1}{2}p\right)|\mathbf{\Sigma}|^{\frac{1}{2}p}\right\}^{-1} |\mathbf{S}|^{\frac{1}{2}(p-n-1)}\mathrm{etr}\left\{-\frac{1}{2}\mathbf{\Sigma}^{-1}\mathbf{S}\right\} \tag{6}$$

Consider that a random symmetric and positive definite matrix $\mathbf{G}$ has mean $\mathbf{G}_0$ and dispersion parameter defined as

$$\delta_G^2 = \frac{\mathrm{E}\left[\|\mathbf{G} - \mathrm{E}[\mathbf{G}]\|_{\mathrm{F}}^2\right]}{\|\mathrm{E}[\mathbf{G}]\|_{\mathrm{F}}^2} \tag{7}$$

$\mathbf{G}$ can be modeled by a Wishart matrix with parameters p and $\mathbf{\Sigma}$ so that $\mathbf{G} \sim W_n(p, \mathbf{\Sigma})$ where $p = n + 1 + \theta$, $\mathbf{\Sigma} = \mathbf{G}_0/\theta$, $\theta = \frac{1}{\delta_G^2}\{1 + \gamma_G\} - (n+1)$ and $\gamma_G = \{\mathrm{Trace}(\mathbf{G}_0)\}^2/\mathrm{Trace}\left(\mathbf{G}_0{}^2\right)$. Based on the theory of Wishart matrices, we have rigorously proved that the eigenvalue density of large stochastic dynamical systems has very strong convergence property. In particular we have shown that the rate of convergence is $O(n^{-2})$.



(a) The finite element model of the Lynx tail boom (b) The density of eigenvalues with random shell thickness variations

Uncertainty quantification using HDMR

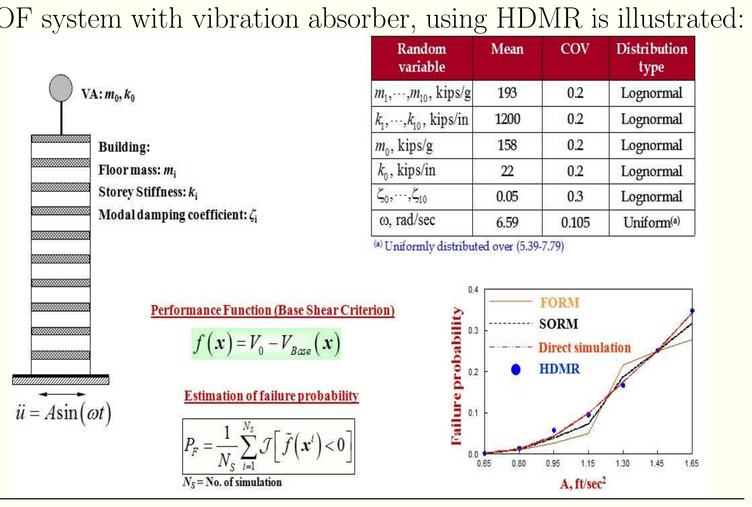
The high dimensional model representation (HDMR) of an arbitrary M-dimensional response function $f(\mathbf{x})$, $\mathbf{x} \in \Re^M$ can be derived by partitioning the identity operator $\mathcal{I}$, to be called $\mathcal{I}_M$ in the M-dimensional case and in the 1D case hereafter, with respect to the projectors $\mathcal{P}_1, \mathcal{P}_2, \ldots, \mathcal{P}_M$ as follows:

$$\begin{aligned}\mathcal{I}_M &= \prod_{m=1}^{M}(\mathcal{P}_m + (\mathcal{I}_1 - \mathcal{P}_m)) \\ &= \underbrace{\prod_{m=1}^{M}\mathcal{P}_m}_{1\text{ term}} + \underbrace{\sum_{m=1}^{M}(\mathcal{I}_1 - \mathcal{P}_m)\prod_{s\neq m}\mathcal{P}_s}_{\binom{M}{1}\text{ terms}} + \\ &\quad + \cdots + \underbrace{\sum_{m=1}^{M}\mathcal{P}_m\prod_{s\neq m}(\mathcal{I}_1 - \mathcal{P}_s)}_{\binom{M}{M-1}\text{ terms}} + \underbrace{\prod_{m=1}^{M}(\mathcal{I}_1 - \mathcal{P}_m)}_{1\text{ term}}\end{aligned} \tag{8}$$

composed of 2^M mutually orthogonal terms. The orthogonal representation of the above is a manifestation of the HDMR and can be rewritten as,

$$\begin{aligned}f(\mathbf{x}) =& \mathcal{L}_{\mathbf{x}}^* + \sum_{i=1}^{M}\mathcal{L}_{\mathbf{x}/x_i}^* + \sum_{i_1=1}^{M}\sum_{i_2=i_1+1}^{M}\mathcal{L}_{\mathbf{x}/x_{i_1}/x_{i_2}}^* \\ &+ \cdots + \sum_{1\leq i_1\leq i_2\leq\cdots\leq i_\alpha}\mathcal{L}_{\mathbf{x}/x_{i_1}/x_{i_2}/\cdots/x_{i_\alpha}}^* + \mathcal{L}_{\mathbf{x}/x_1/x_2/\cdots/x_M}^*\end{aligned} \tag{9}$$

where $\mathcal{L}_{\mathbf{x}}^*$ is a constant term representing the zeroth-order component function or the mean response of any response function $f(\mathbf{x})$, $\mathcal{L}_{\mathbf{x}/x_i}^*$ is the first-order term expressing the effect of variable x_i acting alone, although generally nonlinear, upon the output $f(\mathbf{x})$. The function $\mathcal{L}_{\mathbf{x}/x_{i_1}/x_{i_2}}^*$ a second-order term which describes the cooperative effects of the variables x_{i_1} and x_{i_2} upon the output. The higher order terms gives the cooperative effects of increasing numbers of input variables acting together to influence the output response. Usually the higher order terms in Eq. 9 are negligible such that HDMR with only few low order correlations, amongst the input variables are typically adequate in describing the output behavior resulting in rapid convergence of HDMR expansion. The above HDMR expansion has a finite number of terms and is always exact. Other popular expansions (e.g., polynomial chaos) commonly have an infinite number of terms with some specified functions, such as Hermite polynomials. Estimation of failure probability due to the exceedance of base shear for a 10-DOF system with vibration absorber, using HDMR is illustrated:



Random variable	Mean	COV	Distribution type
$m_1,\cdots,m_{10}$, kips/g	193	0.2	Lognormal
$k_1,\cdots,k_{10}$, kips/in	1200	0.2	Lognormal
m_0, kips/g	158	0.2	Lognormal
k_0, kips/in	22	0.2	Lognormal
$\zeta_0,\cdots,\zeta_{10}$	0.05	0.3	Lognormal
ω, rad/sec	6.59	0.105	Uniform[a]

[a] Uniformly distributed over (5.39-7.79)

Selected Publications

[1] Chowdhury, R., Adhikari, S., and Mitchell, J., "Vibrating carbon nanotube based bio-sensors," *Physica E: Low-Dimensional Systems and Nanostructures*, 2009, published online.
[2] DiazDelaO, F. A. and Adhikari, S., "Structural dynamic analysis using Gaussian process emulators," *Engineering Computations*, 2009, accepted.
[3] Adhikari, S., "Matrix variate distributions for probabilistic structural mechanics," *AIAA Journal*, Vol. 45, No. 7, July 2007, pp. 1748–1762.
[4] Adhikari, S., "Wishart random matrices in probabilistic structural mechanics," *ASCE Journal of Engineering Mechanics*, Vol. 134, No. 12, December 2008, pp. 1029–1044.
[5] Adhikari, S. and Sarkar, A., "Uncertainty in structural dynamics: experimental validation of wishart random matrix model," *Journal of Sound and Vibration*, Vol. 323, No. 3-5, 2009, pp. 802–825.

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