Predictor-Corrector Algorithm with Embedded Dimension Reduction for Uncertainty Quantification of MWCNT On-Chip Interconnect Networks

Surila Guglani and Sourajeet Roy
Department of Electronics and Communication Engineering,
Indian Institute of Technology Roorkee, Roorkee, India
Email: sourajeet.roy@ece.iitr.ac.in

***Abstract* — This paper presents a novel polynomial chaos (PC) approach for the fast uncertainty quantification of on-chip multi-walled carbon nanotube (MWCNT) interconnect networks. The proposed approach combines the benefits of predictor-corrector algorithms with that of dimension reduction strategies to provide two distinct levels of numerical efficiency when training the PC metamodels. As a result, this approach is even better scalable with respect to the number of problem dimensions than conventional predictor-corrector algorithms and state-of-the-art dimension reduction techniques.**

***Keywords* — Interconnect networks, multi-walled carbon nanotubes (MWCNTs), predictor-corrector algorithm, polynomial chaos, uncertainty quantification.**

I. Introduction

As copper interconnects reach their performance limits at the 22 nm technology node, multi-walled carbon nanotube (MWCNT) interconnects are emerging as their potential replacement for on-chip applications [1], [2]. In particular, MWCNT provide longer mean free path of electrons, consequently smaller scattering resistance, greater current carrying capacity, and greater robustness to thermal breakdown than copper interconnects.

Unfortunately, despite the improved performance of MWCNT interconnect networks, they are highly susceptible to fabrication process variations. Therefore, circuit designers must quantify the impact of fabrication process variations on the performance of MWCNT networks at the earliest design stage. Typically, this is done using the brute-force Monte Carlo (MC) technique. However, due to the slow convergence of MC, its computational cost often becomes prohibitively large. This is especially true for MWCNT interconnect networks where the circuit size can be massively large. In such circumstances, the generalized polynomial chaos (PC) technique has been found to be usually more efficient [3], [4]. The PC technique models the impact of fabrication process variations on the MWCNT network responses as a linear expansion of orthonormal basis functions of random variables. This expansion is referred to as a surrogate model or metamodel. The coefficients of the metamodel are the unknowns of the system which are often evaluated using non-intrusive techniques.

A major drawback of the PC technique is that it suffers from the ‘curse of dimensionality’. This means that the number of unknown coefficients in a PC metamodel scales in an exponential manner with respect to the number of random variables (or random dimensions) used to model the fabrication process variations [4], [5]. In turn, the number of deterministic SPICE simulations required to evaluate or ‘train’ these unknown PC coefficients too scale in a similar exponential manner, thereby making the conventional PC technique computationally intractable for large multidimensional problems.

Recently, multiple approaches have been reported to address the poor scalability of PC specifically for MWCNT interconnect networks [4], [5]. For example, the predictor-corrector algorithm improves the scalability by intelligently combining the numerical efficiency of a low-fidelity compact equivalent single conductor (ESC) model with the accuracy of a high-fidelity rigorous multiconductor circuit (MCC) model of the MWCNT network [5]. Another approach is the reduced dimension technique where the PC metamodel is constructed using only the most important random dimensions while other unimportant dimensions are ignored [4].

This work combines, for the very first time, the benefits of both the predictor-corrector algorithm of [5] and the dimension reduction technique of [4]. The proposed approach begins by constructing a predictor PC metamodel trained using the ESC model simulations of the MWCNT network. Next, in order to correct for the errors in the predictor metamodel arising from the approximations in the ESC model, a new corrector PC metamodel is constructed. Typically, the corrector metamodel is trained using MCC model simulations of the MWCNT network. Crucially, the corrector metamodel exploits the correlation between the results obtained from the predictor metamodel and the true MWCNT network responses in order to minimize the number of MCC training simulations that are required in the first place. In this paper, the required number of MCC training simulations is further decreased by ensuring that the corrector metamodel only includes those dimensions which have a large impact on the network responses as inferred from the already trained predictor metamodel. Thus, there exists two

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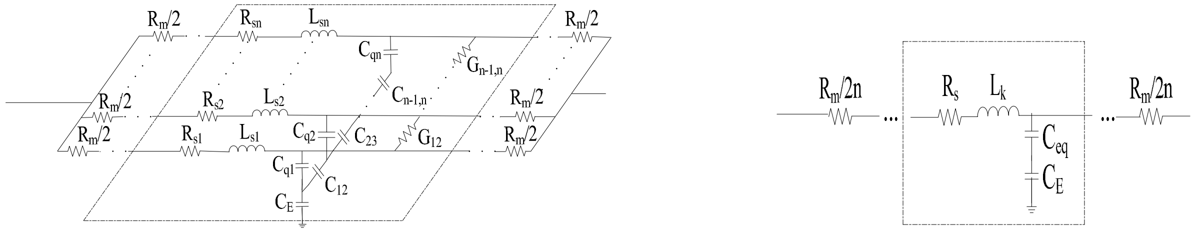

(a) (b)

Fig. 1: MCC and ESC model representations of a MWCNT conductor. Note that the circuit elements inside the box represent an elementary part of the interconnect length and have to be repeatedly cascaded to model the entire conductor length. (a) Multiconductor circuit (MCC) model representation of a MWCNT conductor. (b) Equivalent single conductor (ESC) model representation of a MWCNT conductor.

levels of numerical efficiency when training the proposed corrector leading to relatively more time savings compared to both the conventional predictor-corrector algorithm [5] and existing reduced dimension technique [4]. Note that the proposed approach, in general, can be applied to all types of dimension reduction techniques (e.g., those based on ANOVA, active subspaces or sliced inverse regression). For sake of illustration, in this paper the ANOVA technique using Sobol's sensitivity indices is used for dimension reduction.

II. Development of Proposed approach

Consider a general MWCNT interconnect network consisting of M coupled conductors with N_s number of shells in each conductor. In this case, the electrical behavior of each MWCNT conductor can be accurately represented using the rigorous multiconductor circuit (MCC) model as shown in Fig. 1(a). Let $\boldsymbol{\lambda} = [\lambda_1, \lambda_2, \ldots, \lambda_N]$ be the N-dimensional uncorrelated random variables located within the N-dimensional random space Ω used to represent the fabrication process variations.

A. Developing the Predictor Metamodel

The proposed approach begins by developing a predictor metamodel of the MWCNT network response $x(t,\boldsymbol{\lambda})$ as

$$x_p(t,\boldsymbol{\lambda}) \approx \sum_{k=0}^{P} x_k^{(p)}(t)\phi_k(\boldsymbol{\lambda}) \tag{1}$$

where $x_k^{(p)}(t)$ is the k-th predictor coefficient and $\phi_k(\boldsymbol{\lambda})$ is the k^{th} degree N-dimensional orthonormal polynomial. The number of terms in (1) is truncated to $P+1 = (N+m)!/(N!m!)$, m being the maximum degree of the expansion of (1). The coefficients of (1) are evaluated using SPICE simulations of the ESC model of the MWCNT network. The ESC model is based on the equipotential assumption that has been described in details in [6]. As per the equipotential assumption, all the shells of a conductor will collapse into a single shell as shown in Fig. 1(b). Thus, the ESC model is highly compact when compared to the MCC model and can be solved in SPICE at relatively smaller CPU time costs. In effect, the coefficients of the predictor are trained at very small CPU time costs. However, in reality, the equipotential assumption is an approximation to the MCC model. This means that the basic principle on which the ESC model is based is not perfectly true. Thus, the ESC model will introduce errors into the coefficients of the predictor.

B. Using Predictor to Identify Important Dimensions

The Sobol's sensitivity index of any general i-th dimension can be evaluated as [4]

$$S_i(t) = \frac{\sigma_i^2}{\sigma^2} = \frac{\sigma_i^2}{\sum_{k=1}^{P}(x_k^{(p)}(t))^2} \tag{2}$$

where σ_i^2 is the sum of square of those coefficients whose corresponding basis function has the degree of the univariate polynomial of λ_i greater than zero. The Sobol's sensitivity indices of (2) being time varying quantities, they can be integrated over the entire time window of simulation $[0 - T_{max}]$ to reduce them to scalar quantities. These scalar indices reflect the impact of each dimension on the variance of the network response [4]. Thus, those dimensions whose scalar indices is more than a specific threshold ε, they are considered to be the important dimensions while all other dimensions are considered to be unimportant and can be ignored. In this way, $\boldsymbol{\lambda}$ can be reduced to a vector of N_r important dimensions $\boldsymbol{\xi}$ where $N_r < N$.

C. Developing the Corrector Metamodel

To correct the errors in the predictor metamodel, a corrector PC metamodel is constructed. This corrector metamodel includes only the N_r important dimensions in $\boldsymbol{\xi}$ as

$$f_c(t,\boldsymbol{\xi}) = \sum_{k=0}^{Q} x_k^{(c)}(t)\psi_k(\boldsymbol{\xi}) \approx x(t,\boldsymbol{\lambda}) - x_p(t,\boldsymbol{\lambda}) \tag{3}$$

where $x_k^{(c)}(t)$ is the k-th corrector coefficient and $\psi_k(\boldsymbol{\xi})$ is the k^{th} N_r-dimensional orthonormal polynomial. It is known from [5] that the covariance between the predictor output and the true response of the MWCNT network is usually large, thus making the variance of the corrector metamodel small. This means that only a sparse set of $Q+1$ terms in the corrector is sufficient to capture the error term on the right hand side of (3) where $Q+1 << P+1$. This is the main reason why very few MCC model simulations are sufficient to train the corrector coefficients. In this work, however, the value of $Q+1$ is further decreased by including only the most important N_r dimensions in the

TABLE I

UNCERTAIN NETWORK PARAMETERS WITH NORMAL DISTRIBUTION

No	Uncertain Network Parameters	Mean	% SD
1	D_{in1} (Inner diameter of conductor 1)	2.28 nm	15 %
2	D_{in2} (Inner diameter of conductor 2)		
3	d_1 (Inter-shell distance of conductor 1)	0.34 nm	
4	d_3 (Inter-shell distance of conductor 3)		
5	C_{S1} (Driver capacitance of conductor 1)	0.14 fF	
6	C_{S2} (Driver capacitance of conductor 2)		
7	C_{L1} (Load capacitance of conductor 1)	0.049 fF	
8	C_{L1} (Load capacitance of conductor 1)		
9	w (Separation between conductors)	22 nm	
10	H (Height of dielectric)	50 nm	

corrector metamodel instead of the full N dimensions as done before in [5]. Therefore, the dimension reduction technique accelerates the conventional predictor-corrector algorithm of [5]. In fact, the use of the predictor metamodel in (3) ensures that the proposed methodology is also faster than the existing dimension reduction technique of [4].

D. Recovering the PC metamodel

After the predictor and the reduced dimensional corrector are trained, the original PC metamodel of the network response is recovered as

$$\begin{aligned} x(t,\boldsymbol{\lambda}) &\approx x_p(t,\boldsymbol{\lambda}) + f_c(t,\boldsymbol{\lambda}) \\ &= \sum_{k=0}^{P} x_k^{(p)}(t)\varphi_k(\boldsymbol{\lambda}) + \sum_{k=0}^{Q} x_k^{(c)}(t)\psi_k(\boldsymbol{\lambda}) \end{aligned} \tag{4}$$

The additional terms of the corrector metamodel compensate for the errors in the predictor metamodel arising from the equipotential assumption of the ESC model.

III. NUMERICAL RESULT AND DISCUSSION

In this example, a two conductor (M = 2) MWCNT network is considered. The number of shells in each conductor are N_s = 30. The uncertainty in the network is represented using the N = 10 dimensions described in Table I. Line 1 of the network is excited by a voltage source with a saturated ramp waveform of rise time T_r = 0.1 ps and an amplitude of 1 V. Line 2 is victim line. Four approaches are used for the uncertainty quantification of this network – the proposed approach, the reduced dimensional PC scheme of [4], the conventional predictor-corrector algorithm of [5], and the full-blown PC metamodel trained using SPICE MCC model simulations only. All metamodels use a maximum degree of m = 4. For this example, all those dimensions whose scalar sensitivity indices is below a threshold of ε = 0.05 is considered to be unimportant and their effects ignored. Thus, for this example ξ = [Din_1, d_1, d_2, C_{S1}, C_{L1}, w, H]. The corrector metamodel is constructed in the random space described by these 7 dimensions with the hyperbolic truncation factor u = 0.7. For this example, the time cost of an ESC simulation is roughly 53 ms and that of an MCC simulation is 5.45 seconds.

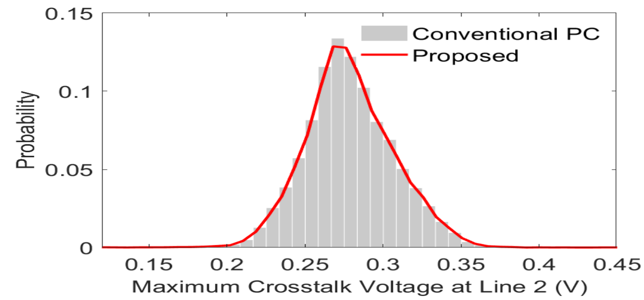

Fig. 2: Histogram depicting the PDF of the peak crosstalk for line 2 obtained using the proposed approach and conventional PC.

TABLE II

CPU TIME FOR NUMERICAL EXAMPLE

	CPU Time (hours)	Speedup w.r.t. Conventional PC
Conventional PC (2002 MCC)	3.03	-
Dimension Reduction PC [4] (654 MCC)	0.99	3.06
Predictor-Corrector Algorithm [5] (2002 ESC + 352 MCC)	0.56	5.41
Proposed (2002 ESC+184 MCC)	0.31	9.83

In this example, the accuracy of the proposed approach is validated by comparing the probability density function of the crosstalk response in Fig. 2. Finally, the CPU training cost for all four aforementioned PC metamodels is recorded and listed in Table II. The results of Table II clearly illustrate the efficiency of the proposed approach.

IV. CONCLUSION

In this paper, a novel PC approach for the fast UQ of MWCNT networks is developed. This approach is numerically far more efficient that both conventional predictor-corrector algorithms as well as existing dimension reduction techniques.

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