Predictor-Corrector Algorithms and Their Scalability Analysis for Fast Stochastic Modeling of Multi-Walled Carbon Nanotube Interconnects

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***Abstract*— In this paper, a predictor-corrector algorithm for the fast stochastic analysis of multi-walled carbon nanotube (MWCNT) interconnect networks is proposed. This algorithm begins by developing a polynomial chaos (PC) predictor metamodel to capture the coarse features in the stochastic network response. In order to expedite the construction of the predictor metamodel, the compact but approximate equivalent single conductor (ESC) model of the network is used. Thereafter, the finer features of the stochastic network response are captured using a corrector metamodel. This corrector metamodel is formulated using a very sparse set of the rigorous and expensive multi-conductor circuit (MCC) model. The combination of the predictor and corrector metamodels is found to be far more efficient than conventional PC metamodels constructed using the MCC model only. In this paper, the scaling of the efficiency factor with respect to the number of shells in the MWCNT network is quantified.**

Keywords — Carbon nanotubes; equivalent single conductor (ESC) model; multi-conductor circuit (MCC) model; polynomial chaos; stochastic analysis

I. Introduction

Multi-walled carbon nanotubes (MWCNTs) are emerging as potential replacements for copper in on-chip high-speed interconnect networks due to their superior electrical and thermal properties [1]-[3]. However, it is pointed out that the performance of MWCNT networks is very sensitive to manufacturing and fabrication process variations. Thus, it is imperative that modern circuit simulators be able to reliably quantify the impact of manufacturing and fabrication process variations on the performance of MWCNT interconnect networks.

Recently, polynomial chaos (PC) approaches have become standard for quantifying the stochastic effects of process variations in high-speed interconnects [4], [5]. These approaches have also been extended to MWCNT networks [6], [7]. The basic idea of any PC approach is to model all process variations as random variables with well-known probability density functions (PDFs). Thereafter, the impact of these input random variables on the response of MWCNT networks is mathematically represented as a linear combination of polynomial basis functions. In particular, these basis functions are, by construction, orthonormal to the joint PDF of the input random variables [8]. Thus, these bases form a set of complete orthonormal bases in the Hilbert space determined by the support of the joint PDF. The coefficients of the bases form the new unknowns of the network. These unknowns are determined using repeated deterministic SPICE simulations of the MWCNT network at predefined points in the multidimensional random space [7]. Once the PC coefficients have been evaluated, the combination of the coefficients and bases form a closed-form metamodel of the network response. This metamodel can now be probed repeatedly to extract the statistics of the response.

The key benefit of PC approaches is their rapid convergence to correct results as the order of the basis functions increases even for massively large number of random variables (or dimensions) [4]-[6]. However, this benefit is counterbalanced by the fact that the number of deterministic SPICE simulations of the MWCNT network required to evaluate the PC coefficients scales in a near-exponential manner with respect to the number of random dimensions [7]. In other words, considering the full set of random dimensions present in a MWCNT network can quickly become computationally intractable. In [6], the approximate but compact equivalent single conductor (ESC) model of the network was harnessed to reduce the burden of each SPICE simulation. However, no approach to compensate for the loss in accuracy caused by the approximate ESC model was explored.

In this paper, a new algorithm to address the poor scalability of PC metamodels specifically for MWCNT networks is presented. This algorithm begins by constructing a predictor PC metamodel of the MWCNT network responses. The main purpose of the predictor is to capture the coarse features of the stochastic network responses. In particular, the massive number of deterministic SPICE simulations required to determine the PC coefficients of the predictor metamodel is mitigated by using the equivalent single conductor (ESC) model of the network [9]. As expected, the ESC model introduces non-negligible errors in the PC coefficients. Next, these non-negligible errors in the predictor coefficients is corrected by adding a corrector function. The corrector function is determined using a very sparse set of the rigorous multiconductor circuit (MCC) model of the network [10]. In other words, the rigor of the MCC model enriches the accuracy

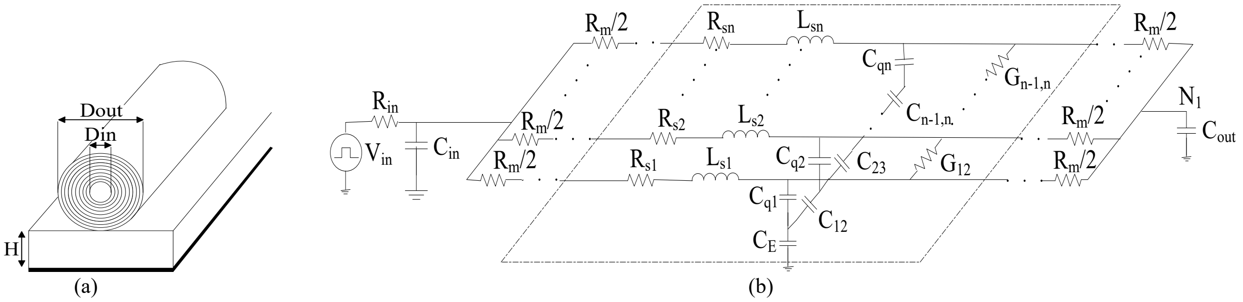


Fig. 1: A MWCNT interconnect network. (a) The MWCNT physical network structure. (b) Multiconductor circuit (MCC) model of the network.

of the predictor metamodel to an acceptable level. Thus, the total number of deterministic SPICE simulations of the MWCNT network required is the sum of a large number of compact ESC model simulations (for constructing the predictor) and a small number of the rigorous MCC model simulations (for constructing the corrector). The CPU cost of this sum of deterministic network simulations is considerably smaller than that incurred when directly constructing a conventional PC metamodel using MCC simulations alone. In this paper, the efficiency achieved by the proposed predictor-corrector algorithm over conventional PC is validated using a numerical example. In addition, complexity analysis quantifying how the achieved efficiency factor scales with respect to the number of conducting shells in the MWCNT network is also presented. The results of this scalability analysis is also validated using the same numerical example.

II. Conventional PC for MWCNT Networks and its Limitation

Consider a typical single conductor MWCNT network structure as shown in Fig. 1(a). The resistance R_{in} and capacitor C_{in} together represent the simple RC equivalent of the interconnect driver while the capacitor C_{out} represents the gate capacitance of the transistor load. Each shell of the conductor is modeled using lumped resistive, inductive, conductive, and capacitive (RLGC) SPICE circuit elements as shown in Fig. 1(b) [3], [10]. Note that in Fig. 1(b), the shell-to-shell coupling is due to the non-zero tunneling conductance and electrostatic capacitance. Overall, Fig. 1(b) represents the rigorous multiconductor circuit (MCC) model of the entire MWCNT network. Let the impact of manufacturing and fabrication process variations in the structure of Fig. 1(a) be modeled as N mutually uncorrelated random variables $\boldsymbol{\lambda} = [\lambda_1, \lambda_2, \ldots, \lambda_N]$ located within the multidimensional support Ω. The impact of the random variables on the MCC model response is characterized by the stochastic modified nodal analysis (S-MNA) equations as

$$\mathbf{G}(\boldsymbol{\lambda})\mathbf{X}(t,\boldsymbol{\lambda}) + \mathbf{C}(\boldsymbol{\lambda})\frac{d\mathbf{X}(t,\boldsymbol{\lambda})}{dt} = \mathbf{B}(t) \quad (1)$$

where $\mathbf{G}$ and $\mathbf{C}$ matrices contain the stamp of all the RLGC lumped circuit elements, $\mathbf{X}$ is the vector of stochastic voltage/current responses, and $\mathbf{B}$ represents the vector of independent voltage and current sources.

The main goal of stochastic analysis is to determine the statistics of the network responses $\mathbf{X}(t,\boldsymbol{\lambda})$. One highly popular and well-known approach for stochastic analysis is using polynomial chaos (PC) metamodels [8]. Typically, PC metamodels express the stochastic network responses $\mathbf{X}(t,\boldsymbol{\lambda})$ as linear combinations of orthonormal basis functions of the random variables of $\boldsymbol{\lambda}$ as [6], [7]

$$\mathbf{X}(t,\boldsymbol{\lambda}) \approx \sum_{k=0}^{P} \mathbf{X}_k(t)\,\phi_k(\boldsymbol{\lambda}) \quad (2)$$

where $\phi_k(\boldsymbol{\lambda})$ is the k^{th} N-dimensional polynomial basis, $\mathbf{X}_k(t)$ is the corresponding coefficient, and the number of terms in the expansion of (2) is truncated to $P+1 = (N+m)!/(N!m!)$, m being the maximum order of the expansion of (2). The unknown PC coefficients of (2) are determined using $K = 2(P+1)$ deterministic SPICE simulations of the MCC model of Fig. 1(b) performed at predetermined points located in the support Ω [7]. Once the coefficients are determined, the PC metamodel of (2) serves as a closed-form surrogate model of the network responses $\mathbf{X}(t,\boldsymbol{\lambda})$. This surrogate model can now be probed repeatedly and far more efficiently than the original MCC model of (1) to estimate the statistical quantities of the network responses $\mathbf{X}(t,\boldsymbol{\lambda})$.

The main computational expense of constructing the PC metamodel of (2) goes towards performing the deterministic SPICE simulations required to evaluate the coefficients. In fact, the number of SPICE simulations required scales rapidly with the number of random dimensions N as $O(K) = O(N^m)$ [7]. This means that even for a modest number of random dimensions N and order m, the required number of SPICE simulations can be too large to be realistically possible. This issue of poor scalability is further compounded by the fact that as the number of shells in each MWCNT conductor increases, the time cost for even a solitary SPICE simulation using the MCC model of Fig. 1(b) increases rapidly. In the work of [6], this issue of poor scalability was mitigated by using the approximate but more compact equivalent single conductor (ESC) model instead of the rigorous MCC model of Fig. 1(b) in each SPICE simulation. However, no methodology for compensate for the reduced accuracy of the approximate ESC model was provided. To address this challenge, a new predictor-corrector algorithm is presented in this paper.

III. Proposed Predictor-Corrector Algorithm

A. Constructing the Predictor Metamodel

The proposed predictor-corrector algorithm begins by constructing a predictor PC metamodel of the MWCNT network responses as

$$\mathbf{X}_{pred}(t,\boldsymbol{\lambda}) \approx \sum_{k=0}^{P} \mathbf{X}_k^{(p)}(t)\,\phi_k(\boldsymbol{\lambda}) \quad (3)$$

where $\mathbf{X}_k^{(p)}(t)$ are the predictor coefficients. The basic purpose of the predictor metamodel of (3) is to capture the coarse features of the stochastic network responses in an efficient manner. To that end, the coefficients of (3) are evaluated using deterministic SPICE simulations based on an ESC model rendering of the MWCNT network [9], [10]. The rationale behind using the ESC model is that it is a highly compact model unlike the rigorous MCC model. Therefore, although a large $K = 2(P+1)$ number of discrete SPICE simulations are required to evaluate all the coefficients of (3), each simulation can be performed substantially faster.

B. Constructing the Corrector Function

It is noted that the ESC model used to evaluate the PC coefficients of (3) is based on the assumption that the potential at all shells of a conductor at equal longitudinal distance from an end is the same [9]. This equipotential assumption neglects the impact of the intershell tunneling conductance and electrostatic capacitance and hence, is an approximation of the underlying physics governing the MWCNT network [10]. In other words, the ESC model is not sufficiently accurate to capture the finer stochastic features of the network responses. In order to restore this lost accuracy of the predictor, a corrector (or error) function is described as

$$\mathbf{F}(t,\boldsymbol{\lambda}) = \mathbf{X}(t,\boldsymbol{\lambda}) - \mathbf{X}_{pred}(t,\boldsymbol{\lambda}) \quad (4)$$

Given that the predictor metamodel is still a reasonably coarse approximation of the actual stochastic network responses, the formulation of (4) indicates that the norm of the variance of the corrector function is significantly lower than that of the responses themselves. Therefore, it is possible to model the corrector function as a low-order PC metamodel as

$$\mathbf{F}(t,\boldsymbol{\lambda}) = \mathbf{X}(t,\boldsymbol{\lambda}) - \mathbf{X}_{pred}(t,\boldsymbol{\lambda}) \approx \sum_{k=0}^{Q} \mathbf{X}_k^{(c)}(t)\,\phi_k(\boldsymbol{\lambda}) \quad (5)$$

where $\mathbf{X}_k^{(c)}(t)$ represents the k^{th} corrector coefficient. In particular, the order of expansion of (5) is r where $r < m$. As a result, the number of coefficients in (5) is $Q+1$ where $Q+1 << P+1$. The coefficients of (5) are evaluated using $2(Q+1)$ discrete SPICE simulations of the rigorous MCC model of Fig. 1(b).

C. Recovering the High-Fidelity PC Metamodel

Once the predictor and corrector have been constructed, the high-fidelity PC metamodel of the MWCNT response can be recovered using (5) as

$$\begin{aligned}\mathbf{X}(t,\boldsymbol{\lambda}) &= \mathbf{F}(t,\boldsymbol{\lambda}) + \mathbf{X}_{pred}(t,\boldsymbol{\lambda}) \\ &\approx \sum_{k=0}^{Q}\left(\mathbf{X}_k^{(c)}(t) + \mathbf{X}_k^{(p)}(t)\right)\phi_k(\boldsymbol{\lambda}) + \sum_{k=Q+1}^{P} \mathbf{X}_k^{(p)}(t)\,\phi_k(\boldsymbol{\lambda})\end{aligned} \quad (6)$$

It is noted from (6) that the addition of the $Q+1$ corrector coefficients restores the accuracy of the predictor metamodel to an acceptable level. In effect, the combination of the predictor and corrector captures both the coarse and fine stochastic features of the network response.

TABLE I
RANDOM PARAMETERS WITH NORMAL DISTRIBUTION FOR NUMERICAL EXAMPLE OF FIG. 1

No.	Random Parameters	Mean	Relative Standard Deviation
1	D_{in} (Inner diameter of CNT)	2.28 nm	20 %
2	d (Inter-shell distance)	0.34 nm	
3	σ (Tunneling conductivity)	20	
4	C_{in} (Driver capacitance)	0.14 fF	
5	C_{out} (Load capacitance)	0.049 fF	
6	H (Height of dielectric)	50 nm	
7	ε_r (Dielectric constant)	2	
8	R_m (Contact resistance)	1000 Ω	
9	l (length of conductor)	100 μm	5 %

D. Computational Complexity Analysis

The main computational cost of the proposed predictor-corrector algorithm is the time cost required for the $2(P+1)$ and $2(Q+1)$ SPICE simulations of the network using the ESC and MCC models respectively. Of these, the time cost for each ESC model simulation is assumed to be a fraction q of the corresponding time cost for each MCC model simulation where $q << 1$. Thus, the equivalent number of MCC model simulations required for the proposed predictor-corrector algorithm is

$$\begin{aligned}N_{proposed} &= 2(P+1)q + 2(Q+1) \\ &\approx 2(Pq+Q+q+1)\end{aligned} \quad (7)$$

On the other hand, the conventional PC metamodel of (2) requires $2(P+1)$ number of MCC model simulations to evaluate all the coefficients. Hence, the efficiency of the predictor-corrector algorithm over conventional PC is quantified as

$$\eta = \frac{2(P+1)}{N_{proposed}} = \frac{P+1}{Pq+Q+q+1} \quad (8)$$

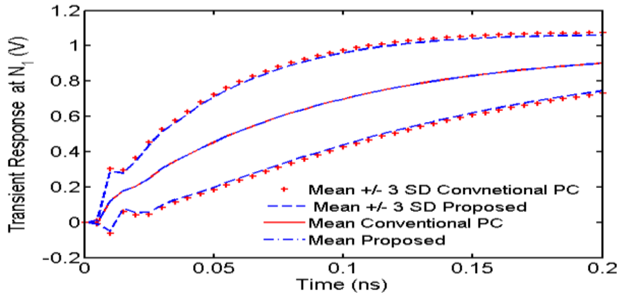
It can be concluded from (8) that as the number of shells inside each MWCNT conductor increases, the ESC model becomes even more efficient than the MCC model. In effect, this means that the value of the reduction factor k decreases with increase in the shell count. For substantially large number of shells, the value of k will be small enough such that the time cost of the ESC model simulations will be dwarfed by the time cost of the MCC model simulations. This will translate to the speedup factor of (8) saturating to the value of

$$\lim_{q\to 0} \eta = \frac{P+1}{Q+1} \quad (9)$$

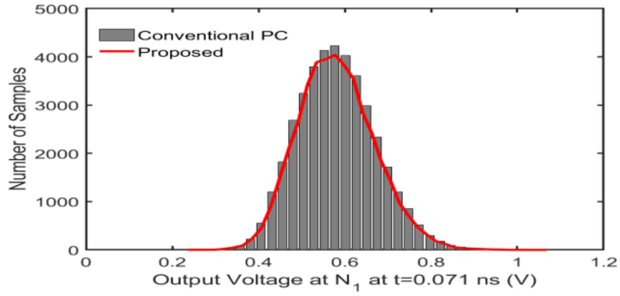
As a result, the best case speedup provided by the predictor-corrector algorithm is $P+1/Q+1$.

IV. NUMERICAL EXAMPLE AND VAIDATION

In order to validate the accuracy and efficiency of the proposed predictor-corrector algorithm, the MWCNT network of Fig. 1 is considered. The number of shells are progressively



(a)



(b)

Fig. 3: Statistics of the transient response at node N_1 of Fig. 1(b). (a) Mean plus/minus three times the standard deviation (SD) of the transient response at node N_1. (b) PDF of the transient response at node N_1 at time point when the SD of the response is maximum (i.e., at t = 0.071 ps).

TABLE II
TIME COST COMPARISON WITH CONVENTIONAL PC

# Shells (n)	Overall Time cost of Predictor-Corrector (s)	Time cost of Conventional PC (s)	Speedup
30	2433.10	11997.70	4.93
40	2502.70	12858.70	5.13
50	2662.20	13678.20	5.14

increased from n = 30 to n = 50 in steps of 10. The uncertainty in the network is represented using N = 9 dimensions described in Table I. The network is excited by a voltage source with a saturated ramp waveform of rise/fall time T_r = 0.1 ps and an amplitude of 1 V. Two different PC based approaches are used for the stochastic analysis of the transient responses of the network – the proposed predictor-corrector algorithm of Section III and the conventional PC metamodel of (2). A maximum degree of m = 4 is used for both the predictor and the conventional PC metamodel. For the corrector, a PC metamodel of order r = 3 is sufficient.

In order to demonstrate the accuracy of the predictor-corrector algorithm, the statistics of the network response at the far end of the network is obtained using the above three methods. The results obtained from the predictor-corrector algorithm are found to exhibit good agreement with the conventional PC results as shown in Fig. 3(a). For a more thorough accuracy analysis, the PDF of the far-end transient response is extracted at the time point when the standard deviation of the same response is maximum (i.e., at t = 0.071 ns). The PDF obtained from the predictor-corrector algorithm also exhibits good agreement with that obtained using the conventional PC approach as shown in Fig. 3(b).

Finally, the time cost incurred by the predictor-corrector algorithm and the conventional PC metamodel of (2) for the three test cases (n = 30, 40, and 50) is reported in Table II. Specifically, for the predictor-corrector algorithm, time costs for the $2(P+1)$ ESC model simulations and the $2(Q+1)$ MCC model simulations are added together to obtain the overall time costs. On the other hand, for the conventional PC metamodel of (2), only the time costs for the $2(P+1)$ MCC model simulations have been listed. All the above model solutions are performed on a workstation with 8 GB RAM, 160 GM memory and an Intel i5 processor with 3.4 GHz clock speed. Note that the speedup achieved in all three test cases is roughly 5x times. This speedup is within 4% of what is expected from the theoretical complexity analysis of (9).

V. CONCLUSION

In this paper, a predictor-corrector algorithm has been developed for the fast stochastic analysis of multi-walled carbon nanotube interconnect networks. This algorithm crosscuts the numerical efficiency of the approximate equivalent single conductor (ESC) model representation with the rigor of the multiconductor circuit (MCC) model representation in order to achieve a far better accuracy-CPU cost tradeoff than that seen in conventional PC metamodels.

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