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## RESEARCH ARTICLE

# A Bilevel Multi-Fidelity Polynomial Chaos Approach for the Uncertainty Quantification of MWCNT Interconnect Networks With Variable Imperfect Contact Resistances

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**ABSTRACT** With on-chip copper interconnects reaching their performance limits at 22 nanometer technology nodes, multi-walled carbon nanotube (MWCNT) interconnects are projected to replace them below this point. A major aspect of MWCNT interconnect design is to perform uncertainty quantification (UQ) in an efficient yet accurate manner. In this paper, a polynomial chaos (PC) based approach is developed for the UQ of MWCNT interconnect networks under the condition that some shells of each conductor of the network are perfectly contacted while others are imperfectly contacted. The key feature of the proposed approach is the development of a bilevel multi-fidelity algorithm where two different low-fidelity models are combined together. The main outcome of using this bilevel approach is to further reduce the computational time cost of state-of-the-art single level multi-fidelity algorithms, especially in the presence of variable imperfect contact resistances where single level multi-fidelity algorithms fail to provide much speedup over conventional PC approaches. The proposed approach adopts a SPICE hybrid model that combines the features of the equivalent single conductor (ESC) model and the rigorous multiconductor circuit (MCC) model of the MWCNT conductors. Then the low-fidelity ESC model, the intermediate-fidelity hybrid model, and the high-fidelity MCC model are exploited in a bilevel multi-fidelity algorithm for the recovery of the PC metamodel of the interconnect network. This proposed bilevel multi-fidelity algorithm is demonstrably 3-5x more numerically efficient than state-of-the-art single level multi-fidelity algorithms while being even more accurate. Once recovered, the PC metamodel is used to derive all statistical information of the network transient responses.

**INDEX TERMS** Imperfect contact resistance, interconnect networks, multi-fidelity algorithms, multi-walled carbon nanotubes (MWCNTs), polynomial chaos, signal integrity, uncertainty quantification.

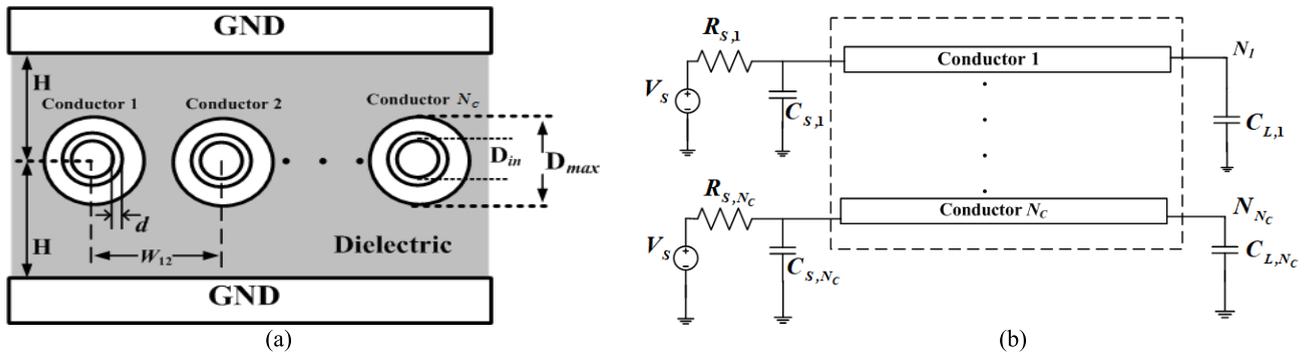
## I. INTRODUCTION

### A. INTRODUCTION

The effective per-unit-length (p. u. l.) resistance of conventional copper on-chip interconnects far exceed their

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bulk value at sub-22 nm technology nodes [1], [2], [3]. This is because of various scattering mechanisms such as sidewall and top/bottom surface scattering, surface roughness scattering, and grain boundary scattering. On the other hand, multi-walled carbon nanotubes (MWCNTs) offer near-ballistic transport, greater thermal conductivity, greater current carrying capacity, and greater mechanical



**FIGURE 1.** Layout and circuit schematic of a general MWCNT interconnect network. (a) Cross-sectional view of the MWCNT conductors. (b) Circuit schematic of the MWCNT interconnect network showing the driver/load circuits.

and electrical reliability than pure copper [4], [5], [6]. Thus, MWCNT interconnects are currently being investigated as promising alternatives to pure copper interconnects for advanced technology nodes. Unfortunately, the performance of MWCNT interconnect networks is highly sensitive to fabrication process variations and manufacturing tolerances [7]. Therefore, there is a strong need to develop reliable uncertainty quantification (UQ) modeling tools for emerging MWCNT interconnect networks.

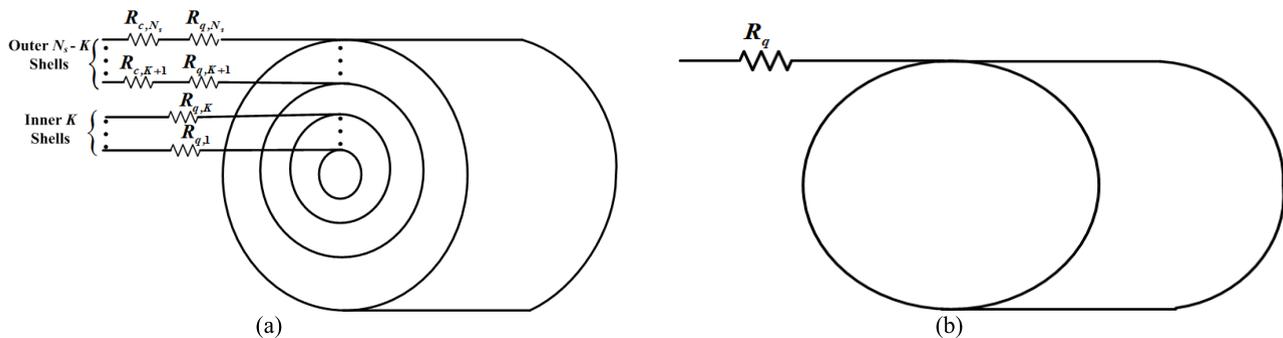
Currently, surrogate modeling or metamodeling techniques such as the generalized polynomial chaos (PC) approach have become the method of choice for the UQ of MWCNT interconnect networks [8], [9], [10], [11], [12]. The PC approach expresses the network transient responses as linear combinations of orthonormal polynomial basis functions of random variables. These random variables model the fabrication process variations and manufacturing tolerances of the network [13]. The coefficients of the basis functions are the unknowns of the network. These coefficients are evaluated using various non-intrusive techniques, all of which require multiple deterministic SPICE simulations of the network [14]. Once these coefficients are determined, the linear combination of basis functions (i.e., the PC metamodels) of the network responses are said to be trained. The trained PC metamodels now serve as closed-form surrogates of the network responses and can be used in a Monte Carlo framework to efficiently extract the response statistics. Unfortunately, the major drawback of the PC approach is that it suffers from the curse of dimensionality [9]. This means that the number of deterministic SPICE simulations required to evaluate the coefficients, and consequently, the time cost for training a PC metamodel scales in a near-exponential manner with respect to the number of random variables (or dimensions) used to represent the fabrication process variations of the MWCNT network [9], [10], [11]. Hence, the UQ of realistically high-dimensional MWCNT interconnect networks can often be computationally intractable.

Several numerical strategies such as compressed sensing [15], [16], dimension and/or basis reduction [17], [18], [19], [20], [21], [22], and multi-fidelity algorithms [10], [11], [12], [23], [24], [25], [26], [27], [28] have been reported to address the curse of dimensionality. Of these, multi-fidelity

algorithms are particularly well-suited for MWCNT interconnect networks [10], [11], [12]. Previous works have demonstrated that multi-fidelity algorithms can crosscut the numerical efficiency of a low-fidelity equivalent single conductor (ESC) model of MWCNTs [29] with the accuracy of a high-fidelity multiconductor circuit (MCC) model to achieve a far better accuracy versus time cost tradeoff when training PC metamodels than what is possible using MCC model simulations alone [10], [11].

It has been shown in the work of [10] that the numerical efficiency of multi-fidelity algorithms is predicated on the correlation between the ESC and the MCC model results of the MWCNT interconnect network under test. Greater the correlation between the ESC and the MCC model results, smaller are the number of SPICE MCC model simulations required to train the PC metamodel, and hence, smaller is the training time cost. Now, for most cases, the ESC model results are well-correlated with the MCC model results. However, one exception to this rule is when there is variation in the imperfect contact resistance of the different shells in a MWCNT conductor [12]. To better understand why this is so, recall that the ESC model collapses the multiple shells of an MWCNT conductor into a single shell where the equivalent imperfect contact resistance of this single shell is the parallel combination of the imperfect contact resistances of all the individual shells. Now, assume that some of the shells of a MWCNT conductor have perfect contacts (i.e., the imperfect contact resistance of these shells is zero) while the remaining shells have imperfect contacts (i.e., the imperfect contact resistance of these shells is non-zero). In this case, the equivalent imperfect contact resistance of the ESC model will be equal to zero. As a result, the ESC model will implicitly ignore the signal losses across all the non-zero imperfect contact resistances of the conductor. This incorrect treatment of the imperfect contact resistances weakens the otherwise strong correlation existing between the ESC and MCC model results of the network. In such scenarios, conventional multi-fidelity algorithms usually fail to provide any numerical efficiency [12].

In this paper, the above loss in numerical efficiency of conventional multi-fidelity algorithms caused by the variation in the imperfect contact resistances of different shells of a



**FIGURE 2.** Treatment of variable imperfect contact resistances in an MWCNT conductor by the ESC model. (a) Arrangement of shells in the MWCNT conductor where the inner  $K$  shells are perfectly contacted and the outer  $N_s - K$  shells are poorly contacted. (b) ESC model representation of the MWCNT conductor where the imperfect contact resistances are treated incorrectly.

MWCNT conductor is addressed. This work is based on the authors preliminary work of [12] where a new hybrid model of MWCNT conductors was introduced. The hybrid model, as the name suggests, combined features of the known ESC and MCC models. In so doing, the hybrid model enabled a more correct treatment of the contact resistances in MWCNT conductors than the original ESC model, and hence, enjoyed a better correlation with respect to the MCC model results. This improved correlation was used to ensure that the multi-fidelity algorithm of [12] was able to offer some numerical efficiency when training the PC metamodel. ext.

## B. CONTRIBUTIONS AND RELATED WORKS

In this paper, additional new contributions above and beyond the works of [10], [11], [12] are presented as follows:

(i) In this paper, a fundamental limitation of the multi-fidelity algorithm of [12] arising from the relatively large SPICE simulation cost of the hybrid model compared to the ESC model is highlighted. In fact, through multiple numerical examples in Section IV of this paper, it is demonstrated that because of the relatively large SPICE simulation cost of the hybrid model, the approach of [12] is able to achieve only marginal numerical efficiency when training PC metamodels. Importantly, this limitation has not been examined in [12].

(ii) In this paper, a novel bilevel multi-fidelity algorithm is developed to address the poor numerical efficiency of the approach of [12]. At the first level of the bilevel approach, a multi-fidelity algorithm will crosscut the numerical efficiency of the ESC model of MWCNT interconnects with the relative greater accuracy of the hybrid model to expedite the training of a predictor PC metamodel. In the second level, another multi-fidelity algorithm will crosscut the relative numerical efficiency of the hybrid model with the greater accuracy of the rigorous MCC model to expedite the training of a corrector PC metamodel. The sum of the predictor and corrector metamodels will recover the original PC metamodel of the network responses. The key advantage of the proposed bilevel multi-fidelity algorithm will be to ensure that significantly high amounts of numerical efficiency is achieved in training not only the corrector metamodel (as in [12]) but the

predictor metamodel as well (not possible in [12]). Thus, this bilevel approach will provide an additional level of numerical efficiency not seen in existing single level multi-fidelity algorithms of [10], [11], [12]. Remarkably, in Section IV of this paper, the bilevel approach is also found to be much more accurate than existing single level multi-fidelity algorithms [10], [11], [12] – a bonus benefit of this work.

(iii) At this point, it is emphasized that the proposed bilevel multi-fidelity algorithm differs from the two-level multi-fidelity algorithm of [11] in the sense that the work of [11] uses a multi-fidelity algorithm at only the first level. The second level of [11] uses a dimension reduction technique. Therefore, [11] is simply a single level multi-fidelity formulation. In contrast, the proposed approach uses multi-fidelity at two distinct levels – something only possible using the new hybrid SPICE model of the conductors of [12] not seen in [11]. Another point of contrast is that this work is specifically for the case where there is variation in the imperfect contact resistance of different shells in an MWCNT conductor whereas in [11] no variability in the imperfect contact resistance is considered.

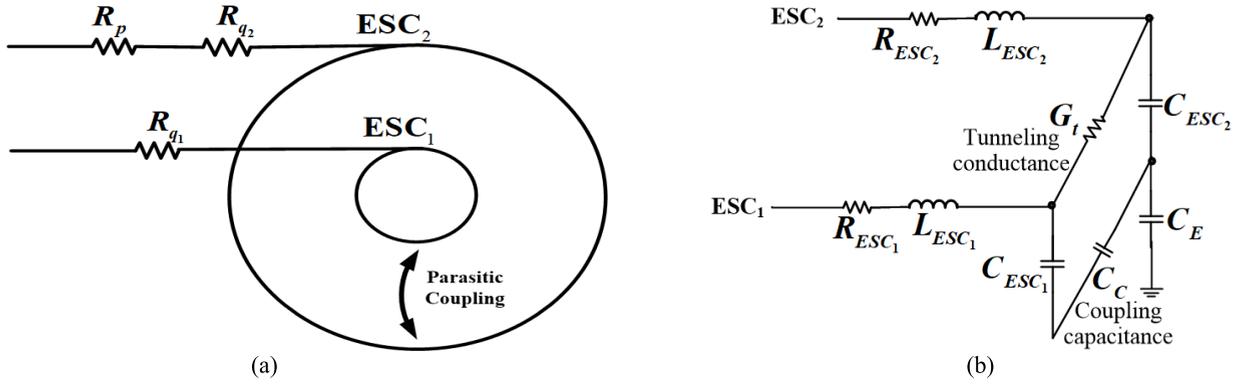
(iv) In this work, a mathematically rigorous estimate of the maximum numerical efficiency achieved by the proposed bilevel multi-fidelity algorithm over existing single level multi-fidelity algorithms is presented. These efficiency bounds are validated via multiple numerical examples.

The paper is organized as follows. Section II explains the problem statement. Section III provides the description of the proposed bilevel multi-fidelity algorithm and also compares its computational complexity with that of conventional single level multi-fidelity algorithms. Finally, Section IV presents two numerical examples for validation of the proposed approach followed by conclusions in Section V.

## II. PROBLEM STATEMENT

### A. CONVENTIONAL MULTI-FIDELITY ALGORITHMS FOR MWCNT INTERCONNECT NETWORKS

Let the parametric uncertainty in the MWCNT interconnect network of Fig. 1 be modeled by  $N$  mutually uncorrelated random variables  $\lambda = [\lambda_1, \lambda_2, \dots, \lambda_N]$  located within the



**FIGURE 3.** Treatment of variable imperfect contact resistances in an MWCNT conductor by the hybrid model. (a) The hybrid model decomposing an MWCNT conductor into two ESC models. (b) The circuit schematic of the two ESC models making up the hybrid model.

multidimensional support  $\Omega$ . Now, due to the uncertainty in the network parameters, the transient response of the network, say  $x(t, \lambda)$ , will be uncertain as well where  $t$  is the temporal variable. In order to extract the statistics of the uncertain response, a PC metamodel of the response need to be constructed. One highly efficient approach to train the PC metamodel is to employ the conventional multi-fidelity algorithm. As per this algorithm, initially a predictor PC metamodel of the response is constructed as [12]

$$x_p(t, \lambda) \approx \sum_{k=0}^{N_0} x_k^{(p)}(t)\phi_k(\lambda); N_0 + 1 = \frac{(N + m)!}{N!m!} \quad (1)$$

where  $x_k^{(p)}(t)$  is the  $k$ -th predictor coefficient,  $\phi_k(\lambda)$  is the  $k$ -th  $N$ -dimensional multivariate orthonormal basis function, and the total number of terms in the PC expansion of (1) is  $N_0$  with the maximum order of expansion being equal to  $m$ . The predictor metamodel of (1) is trained by harnessing the data elicited from the SPICE simulations of the approximate but compact ESC model of the network of Fig. 1 and then using this data in a non-intrusive approach [10]. Recall that the ESC model is based on an equipotential approximation of a MWCNT conductor whereby all the shells of each conductor of Fig. 1(a) collapses into a single shell [29]. Thus, the equipotential approximation of the ESC model ensures that it is significantly cheaper to simulate than the rigorous and cumbersome MCC model. In return, the errors arising from the equipotential approximation reduces the accuracy of the ESC model. This loss of accuracy translates to the predictor metamodel of (1) being able to only capture the coarse statistical features of the network response. Now, the errors in the predictor metamodel of (1) stemming from the equipotential approximation of the ESC model can be compensated by a corrector function described as [10]

$$f_c(t, \lambda) = x(t, \lambda) - x_p(t, \lambda) \quad (2)$$

Equation (2) shows that the corrector function captures the finer statistical features of the response  $x(t, \lambda)$  that the predictor metamodel has missed. This corrector function is also

represented as a PC metamodel as

$$f_c(t, \lambda) = \sum_{k=0}^Q x_k^{(q)}(t)\phi_k(\lambda) \quad (3)$$

where  $x_k^{(q)}(t)$  is the  $k$ -th corrector coefficient. Because the corrector has to capture only the finer statistical features of the response  $x(t, \lambda)$  instead of the whole response, a very sparse set of PC terms in (3) is sufficient. In other words, the number of terms (or coefficients)  $Q + 1 \ll N_0 + 1$  of the predictor metamodel of (1). To evaluate these few coefficients, very few SPICE simulations of the rigorous MCC model are required. This is exactly why multi-fidelity algorithms can train PC metamodels much more efficiently than standard techniques. Finally, adding the predictor and corrector metamodels of (1) and (3) together recovers the original PC metamodel of the network response.

From the formulation of the corrector in (2), it is noted that the variance of the corrector is given as

$$Var(f_c) = Var(x) + Var(x_p) - 2Cov(x_p, x) \quad (4)$$

Equation (4) indicates that greater the correlation between the predictor metamodel result  $x_p(t, \lambda)$  and the true network response  $x(t, \lambda)$ , smaller will be the variance of the corrector, and hence, smaller will be the number of terms required (i.e.,  $Q + 1$ ) to model the corrector in (3). This, in turn, will suppress the number of SPICE simulations of the MCC model required to train the corrector metamodel. Thus, the correlation between the ESC and the MCC model results controls the numerical efficiency of the multi-fidelity algorithm [10]. When there is no variability present in the imperfect contact resistances, the correlation between the ESC and the MCC model results is reasonably strong leading to very fast training of the corrector metamodel [10]. However, when variability is present in the imperfect contact resistances, the correlation between the ESC and MCC model results weakens, thereby requiring an inordinately large number of MCC model simulations to train the corrector metamodel of (3), as explained next.

**B. EFFECT OF IMPERFECT CONTACT RESISTANCES ON MULTI-FIDELITY ALGORITHMS**

Consider the MWCNT interconnect network of Fig. 1 where now for each conductor, the inner  $K$  shells are perfectly contacted to the metal electrode while the outer  $N_s - K$  shells are poorly contacted. This means that the values of the imperfect contact resistance of the shells are given as

$$R_{c,i} = 0; 1 \leq i \leq K \gg 0; K + 1 \leq i \leq N_s \quad (5)$$

where  $R_{c,i}$  is the imperfect contact resistance of the  $i$ -th shell and  $N_s$  is the total number of shells in the MWCNT conductor. In addition to the imperfect contact resistance, each  $i$ -th shell also has a quantum contact resistance given as [7], [8]

$$R_{q,i} = \frac{h}{2e^2 N_{ch,i}}; 1 \leq i \leq N_s \quad (6)$$

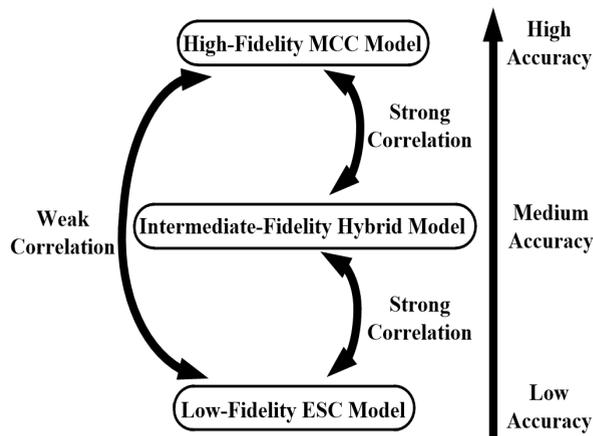
where  $h$  is the Planck’s constant,  $e$  is the charge of an electron, and  $N_{ch,i}$  is the number of conducting channels in the  $i$ -th shell. The total contact resistances of the different shells are shown in detail in Fig. 2(a). In such a scenario, the ESC model dictates that the  $N_s$  shells of the conductor collapse into a single shell as shown in Fig. 2(b). Importantly, for the single shell, the equivalent imperfect contact resistance is the parallel combination of all the imperfect contact resistances of the individual shells in Fig. 2(a) and is expressed as [8]

$$R_c = \left( \sum_{i=1}^{N_s} (R_{c,i})^{-1} \right)^{-1} \quad (7)$$

Note that because the imperfect contact resistance of the inner  $K$  shells is equal to zero (i.e.,  $R_{c,i} = 0$  for  $i \leq K$ ), this makes the equivalent imperfect contact resistance of the single shell in (7) equal to zero as well (see Fig. 2(b)). Similarly, the equivalent quantum contact resistance of the single ESC shell in Fig. 2(b) is the parallel combination of all the quantum contact resistances of the individual shells in Fig. 2(a) and is expressed as [8]

$$R_q = \left( \sum_{i=1}^{N_s} (R_{q,i})^{-1} \right)^{-1} \quad (8)$$

Physically, what this means is that in the ESC model, the signal losses across the imperfect contact resistance of the outer  $N_s - K$  poorly contacted shells are neglected. In other words, the ESC model overestimates the total signal strength entering the MWCNT conductors. The modeling errors stemming from the overestimation of the signal strength entering the conductors is in addition to the errors already due to the equipotential approximation. As a result, the ESC model suffers from additional loss of accuracy when dealing with MWCNT conductors with variable imperfect contact resistance. This additional model inaccuracy significantly weakens the correlation between the ESC and MCC model results as shown in [12]. Consequently, the variance of the corrector in (4) is much higher than expected leading to a greater number of terms required in the metamodel of (3)



**FIGURE 4.** The relative accuracy of the ESC, hybrid, and MCC models and the strength of the correlations between them.

and more SPICE simulations of the MCC model for training. This, in turn, reduces the numerical efficiency possible from the multi-fidelity algorithm [12].

**III. PROPOSED BILEVEL MULTI-FIDELITY ALGORITHM**

**A. REVIEW OF HYBRID MODEL**

In the work of [12], a new SPICE hybrid model for MWCNT interconnect networks is developed by combining the features of the ESC and MCC models. To better explain this hybrid model, the MWCNT interconnect network of Fig. 1 is considered where the imperfect contact resistance of each conductor is as described in Section II-B and Fig. 2. Now, the inner  $K$  shells of each conductor are collectively modeled using an ESC model while the remaining outer  $N_s - K$  shells are collectively modeled using another ESC model. In effect, the conductor is now decomposed into two ESC models. These two ESC models are coupled together via the tunneling conductance and the electrostatic intershell capacitance between the  $K$  and  $K + 1$ -th inner shells as shown in Fig. 3. These coupling circuit elements are exactly the same as those used in the MCC model representation of the conductor. Hence, the proposed model includes attributes of both the ESC and MCC models and is referred to as the hybrid model.

A characteristic feature of the hybrid model is that the imperfect contact resistance of the ESC model representing the inner  $K$  shells does not in any way affect the imperfect contact resistance of the ESC model representing the outer  $N_s - K$  shells. Hence, in this model, the signal losses across the imperfect contact resistances of the outer  $N_s - K$  shells are not ignored unlike the conventional ESC model. In this way, the hybrid model of Fig. 3(a) is able to avoid the incorrect treatment of the imperfect contact resistances observed in the ESC model of Fig. 2(b). Consequently, the hybrid model offers much higher accuracy than the ESC model when dealing with MWCNT conductors suffering from variability in the imperfect contact resistances. This improved accuracy translates to stronger correlation between the hybrid and MCC model results. Therefore, when the hybrid model replaces the ESC model while training the predictor metamodel of the

network response in (1), the loss of numerical efficiency of conventional multi-fidelity algorithms is remedied [12].

However, it is worthwhile to understand that the higher accuracy of the hybrid model relative to the ESC model comes at the price of greater SPICE simulation time costs. This is because the hybrid model treats each MWCNT conductor as two coupled ESC models instead of a single ESC model. Thus, training the predictor metamodel of (1) using repeated solutions of the hybrid model in SPICE will be much more time intensive than using repeated solutions of the ESC model. Consequently, the advantage of greater correlation between the hybrid and MCC model results will be undercut by the greater training time costs of the predictor metamodel, thereby leading to poor numerical efficiency for the approach of [12].

As a concluding remark, it is noted that the hybrid model will collapse the  $N_s$  shells of the MCC model into two shells only. Hence, the time cost of simulating the hybrid model will still be significantly lower than that of simulating the rigorous MCC model. Overall, the accuracy and the concomitant CPU time cost of SPICE simulation for the ESC, hybrid, and MCC models can be ranked as in Fig. 4.

**B. PROPOSED BILEVEL MULTI-FIDELITY ALGORITHM**

In order to reduce the relatively high training time cost of the predictor metamodel of (1) caused by the higher simulation time cost of the hybrid model, in this paper a bilevel multi-fidelity algorithm is developed. The basic idea behind the proposed bilevel algorithm is that instead of directly training the predictor metamodel of (1) using repeated SPICE simulations of the relatively costly hybrid model as in [12], it would be more numerically efficient to employ a second multi-fidelity algorithm based on the ESC model to accelerate this training. For this purpose, at the first level of the bilevel multi-fidelity algorithm, a predictor PC metamodel of the network response will be constructed as [10]

$$x_1(t, \lambda) \approx \sum_{k=0}^{N_0} x_k^{(1)}(t)\phi_k(\lambda) \tag{9}$$

where  $x_k^{(1)}(t, \lambda)$  is the  $k$ -th coefficient of the metamodel. The job of the predictor metamodel of (9) is to capture the coarse statistical features of the network response at the least possible computational time cost. To that end, results of the compact ESC model simulations will be utilized to train the predictor metamodel of (9). Unfortunately, the numerical efficiency provided by the ESC model is counterbalanced by the relatively low accuracy of the model (see Fig. 4). Therefore, to compensate for the errors in the ESC model simulations, a first level corrector function will be defined as the error between the response obtained from the more accurate hybrid model and the predictor metamodel. Mathematically, this corrector function will be represented as a sparse PC metamodel as [10]

$$f_{c_1}(t, \lambda) = x_{hybrid}(t, \lambda) - x_1(t, \lambda);$$

**TABLE 1. Uncertain parameters (normal distribution) for example 1.**

No.	Uncertain Network Parameters	Mean	% SD
1-3	$D_{in1} - D_{in3}$ (Inner diameters of conductors 1-3)	2.28 nm	15 %
4-6	$d_1 - d_3$ (Inter-shell distances of conductors 1-3)	0.34 nm	
7-9	$C_{S1} - C_{S3}$ (Driver capacitances of conductors 1-3)	0.14 fF	
10-12	$C_{L1} - C_{L3}$ (Load capacitances of conductors 1-3)	0.049 fF	
13	$w_{12}$ (Separation between conductors 1 - 2)	22 nm	
14	$w_{23}$ (Separation between conductors 2 - 3)		
15	$H$ (Height of conductors above GND plane)	50 nm	

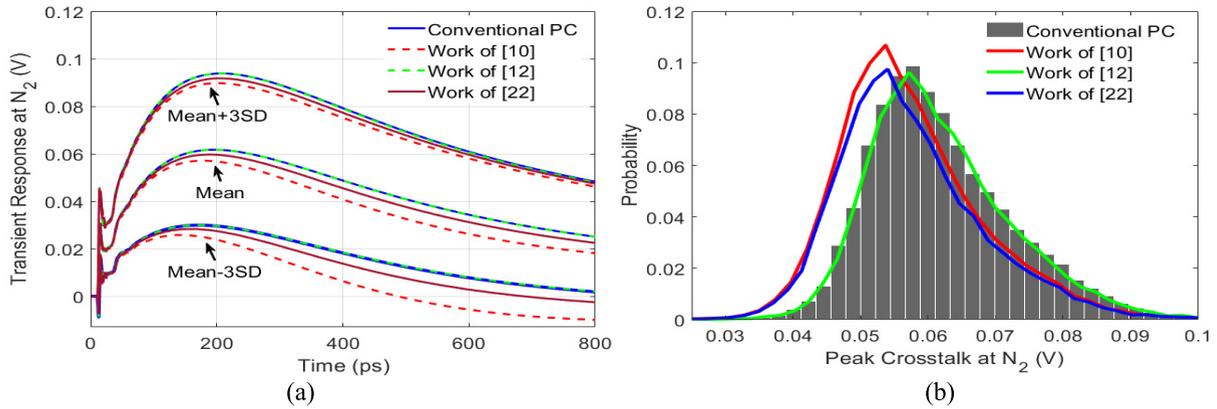
$$= \sum_{k=0}^{\bar{Q}} x_k^{(c_1)}(t)\phi_k(\lambda) \tag{10}$$

where  $x_{hybrid}(t, \lambda)$  is the response of the hybrid model and  $x_k^{(c_1)}(t, \lambda)$  is the  $k$ -th coefficient of the corrector metamodel. From (10), the following points are noted. First, the coefficients of the corrector metamodel can be inferred using any non-intrusive approach via repeated SPICE simulations of the hybrid model. Second, the results of the hybrid model will be well correlated with the results of the ESC model as shown in Fig. 4. Hence, according to (4), the variance of the corrector function will be much smaller than the variance of the response of the hybrid model  $x_{hybrid}(t, \lambda)$ . This means that the number of terms in the corrector metamodel, and consequently, the number of SPICE hybrid model simulations required for training the coefficients of (10) will be much less than the full number of terms required (i.e.,  $\bar{Q} + 1 \ll N_0 + 1$ ). The optimal value of  $\bar{Q} + 1$  can be obtained using the iterative adaptation of the hyperbolic PC expansion described in [12]. Finally, once the corrector metamodel of (10) has been trained, the response of the hybrid model will be recovered as the sum of metamodels [10]

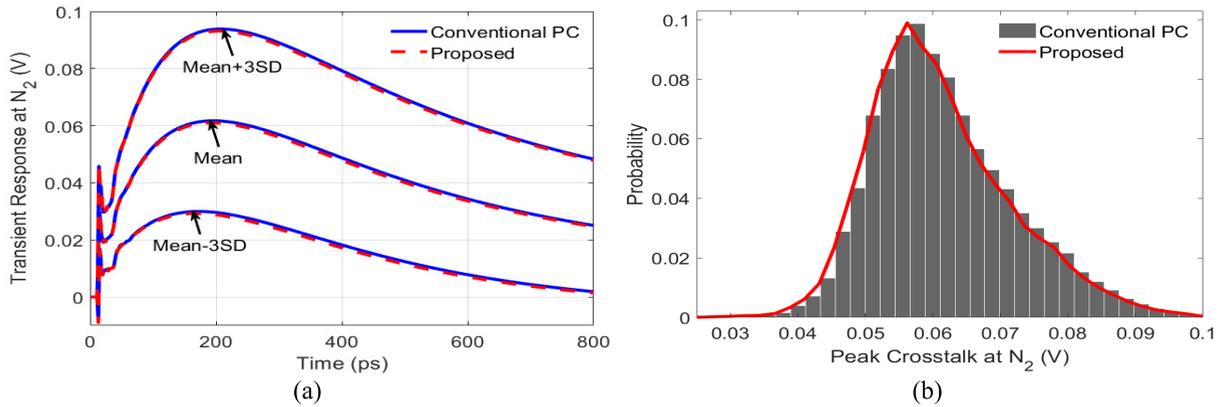
$$\begin{aligned} x_{hybrid}(t, \lambda) &= x_1(t, \lambda) + f_{c_1}(t, \lambda); \\ &= \sum_{k=0}^{N_0} x_k^{(1)}(t)\phi_k(\lambda) + \sum_{k=0}^{\bar{Q}} x_k^{(c_1)}(t)\phi_k(\lambda); \\ &= \sum_{k=0}^{\bar{Q}} \left( x_k^{(c_1)} + x_k^{(1)} \right) \phi_k(\lambda) + \sum_{k=\bar{Q}+1}^{N_0} x_k^{(1)}(t)\phi_k(\lambda) \end{aligned} \tag{11}$$

In this way, via the first level of the multi-fidelity algorithm, the time cost to train the corrector of (10), and consequently to recover the metamodel of (11), will be substantially reduced from the original time cost reported in [12] where the full set of  $N_0 + 1$  simulations of the hybrid model are needed.

Once the PC metamodel of the response of the hybrid model is obtained from (11), the next step is to use the



**FIGURE 5.** Statistics of the transient responses at node  $N_2$  of Example 1. (a) Mean, mean plus three times the SD, and mean minus three times the SD at node  $N_2$  computed using the PC metamodel trained by the single level multi-fidelity algorithm of [10], the single level multi-fidelity algorithm of [12], the hyperbolic PC expansion of [22], and the conventional PC metamodel. (b) PDF of the peak crosstalk at node  $N_2$  computed using the PC metamodel trained by the single level multi-fidelity algorithm of [10], the single level multi-fidelity algorithm of [12], the hyperbolic PC expansion of [22], and the conventional PC metamodel.



**FIGURE 6.** Statistics of the transient responses at node  $N_2$  of Example 1. (a) Mean, mean plus three times the SD, and mean minus three times the SD at node  $N_2$  computed using the PC metamodel trained by the proposed bilevel multi-fidelity algorithm and the conventional PC metamodel. (b) PDF of the peak crosstalk at node  $N_2$  computed using the PC metamodel trained by the proposed bilevel multi-fidelity algorithm and the conventional PC metamodel.

metamodel of (11) as a starting point to obtain a PC metamodel of the true response of the MWCNT interconnect network. This refers to the second level of our multi-fidelity algorithm. In the second level, the metamodel of (11) will serve as the predictor and a corrector function will be described to be the difference between the true response of the network and the response obtained from the hybrid model. This corrector function will take the form

$$f_{c_2}(t, \lambda) = x(t, \lambda) - x_{hybrid}(t, \lambda) \quad (12)$$

where the last term  $x_{hybrid}(t, \lambda)$  will already be known from (11). This second-level corrector function will be modeled using a PC metamodel

$$f_{c_2}(t, \lambda) \approx \sum_{k=0}^R x_k^{(c_2)}(t) \phi_k(\lambda) \quad (13)$$

where  $x_k^{(c_2)}(t, \lambda)$  is the  $k$ -th coefficient of the metamodel. Now, by equating (13) with (12), the coefficients of (13) can be trained non-intrusively. At each regression point, the

true response  $x(t, \lambda)$  will be obtained from a SPICE MCC simulation while the response  $x_{hybrid}(t, \lambda)$  will be known from (11). Moreover, the optimal number of terms required in the second level corrector (i.e.,  $R + 1$ ) will be obtained using the iterative adaptation of the hyperbolic PC expansion described in [10]. Again, because of the strong correlation between the results of the hybrid model and the MCC model (see Fig. 4), the number of SPICE MCC model simulations required for training the corrector metamodel of (13) will be very small (i.e.,  $R + 1 \ll N_0 + 1$ ). Finally, once the second level corrector metamodel has been trained, the overall PC metamodel of the transient response will be recovered as the sum

$$\begin{aligned} x(t, \lambda) &= x_{hybrid}(t, \lambda) + f_{c_2}(t, \lambda); \\ &= \sum_{k=0}^{\bar{Q}} \left( x_k^{(c_1)} + x_k^{(1)} \right) \phi_k(\lambda) + \sum_{k=\bar{Q}+1}^{N_0} x_k^{(1)}(t) \phi_k(\lambda) \\ &\quad + \sum_{k=0}^R x_k^{(c_2)}(t) \phi_k(\lambda); \end{aligned}$$

TABLE 2. Computational time cost for numerical example 1.

	# ESC model simulations	# Hybrid ESC-MCC model simulations	# MCC model simulations	CPU time cost	$L_2$ error norm of SD at node $N_2$ w. r. t. conventional PC	Speedup w. r. t. Conventional PC
Conventional PC	0	0	6120	14 hours 8 minutes	-	-
Single level multi-fidelity algorithm of [10] ( $u = 0.8$ )	6120	0	1388	3 hours 23 minutes	0.124	4.21
Single level multi-fidelity algorithm of [12] ( $u = 0.8$ )	0	6120	1388	4 hours 14 minutes	0.012	3.33
Reduced Dimensional PC of [18]	0	0	2800	6 hours 26 minutes	0.014	2.19
Proposed bilevel multi-fidelity algorithm with $(u_1, u_2) = (0.8, 0.5)$	6120	1388	256	58.8 minutes	0.009	14.41

$$\begin{aligned}
 &= \sum_{k=0}^R \left( x_k^{(c_1)} + x_k^{(c_2)}(t) + x_k^{(1)} \right) \phi_k(\lambda) \\
 &+ \sum_{k=R+1}^{\bar{Q}} \left( x_k^{(c_1)} + x_k^{(1)} \right) \phi_k(\lambda) \\
 &+ \sum_{k=\bar{Q}+1}^{N_0} x_k^{(1)}(t) \phi_k(\lambda) \tag{14}
 \end{aligned}$$

At this juncture, it is pointed out that the proposed bilevel multi-fidelity algorithm will accelerate the recovery of both the predictor metamodel of (11) and the PC metamodel of (14). This is in contrast to the single level multi-fidelity algorithm of [12] which only accelerates the training of the corrector metamodel of (13), and consequently the recovery of the metamodel of (14). Thus, the proposed bilevel multi-fidelity algorithm achieves one additional level of numerical efficiency not possible in the work of [14].

C. COMPUTATIONAL COMPLEXITY ANALYSIS

Let the average SPICE simulation cost of the ESC, hybrid, and MCC models be  $C_1$ ,  $C_2$ , and  $C_3$ , respectively where  $C_1 < C_2 < C_3$ . Based on this knowledge and the equations (9)-(14), the total training time cost of the proposed bilevel multi-fidelity algorithm is quantified as

$$C_{prop} = (N_0 + 1) C_1 + (\bar{Q} + 1) C_2 + (R + 1) C_3 \tag{15}$$

provided the stochastic testing algorithm or the SPLINER approach is used [30], [31]. Similarly, for the single level multi-fidelity algorithm using the hybrid model in [12], the total training cost is quantified as

$$C_{hybrid} = (N_0 + 1) C_2 + (R + 1) C_3 \tag{16}$$

Finally, the training cost for a conventional PC metamodel trained only using MCC simulations is

$$C_{PC} = (N_0 + 1) C_3 \tag{17}$$

TABLE 3. Uncertain parameters (normal distribution) for example 2.

No.	Uncertain Network Parameters	Mean	% SD
1-5	$D_{in1} - D_{in5}$ (Inner diameters of conductors 1-5)	2.28 nm	15 %
6-10	$d_1 - d_5$ (Inter-shell distances of conductors 1-5)	0.34 nm	
11-15	$C_{S1} - C_{S5}$ (Driver capacitances of conductors 1-5)	0.14 fF	
16-20	$C_{L1} - C_{L5}$ (Load capacitances of conductors 1-5)	0.049 fF	

Note that in (15)-(17), the implicit assumption is that the simulation costs of the ESC, hybrid, and MCC models in SPICE dominates over the cost of solving the linear system of equations required in the stochastic testing algorithm or the SPLINER approach to evaluate the PC coefficients [30], [31]. Under these circumstances, the speedup in the training costs provided by the proposed bilevel multi-fidelity algorithm over the conventional PC metamodel is given as

$$\begin{aligned}
 \eta_{prop-PC} &= \frac{C_{PC}}{C_{prop}} \\
 &= \frac{(N_0 + 1) C_3}{(N_0 + 1) C_1 + (\bar{Q} + 1) C_2 + (R + 1) C_3} \tag{18}
 \end{aligned}$$

Now, under the assumptions that the time cost for training the second level corrector of (13) using MCC model simulations far outweighs the time cost for training the first level predictor of (9) using ESC model simulations (i.e.,  $(N_0 + 1)C_1 \ll (R + 1)C_3$ ), the maximum bound of the speedup of (18) can be quantified as

$$\max(\eta_{prop-PC}) = \frac{(N_0 + 1) C_3}{(\bar{Q} + 1) C_2 + (R + 1) C_3} \tag{19}$$

A similar analysis leads to the following quantification of the maximum bound of the speedup achieved by the proposed bilevel multi-fidelity algorithm over the single level

multi-fidelity algorithm of [12]

$$\max(\eta_{prop-hybrid}) \approx \frac{(N_0 + 1) C_2 + (R + 1) C_3}{(\bar{Q} + 1) C_2 + (R + 1) C_3} \quad (20)$$

It is important to note that the speedup of (20) is always more than 1 given that  $\bar{Q} + 1 \ll N_0 + 1$  due to the utilization of the first-level of the proposed multi-fidelity algorithm. This proves that the proposed bilevel multi-fidelity algorithm will outperform the single level multi-fidelity algorithm of [12] although both use the same hybrid model – the central contribution of this paper. Next, the results of (19) and (20) are validated using various numerical examples.

#### IV. NUMERICAL EXAMPLES

In this section, two numerical examples are presented to demonstrate the benefits of the proposed bilevel multi-fidelity algorithm over existing single level multi-fidelity algorithms of [10], [12] and other fast non-multi-fidelity approaches when dealing with MWCNT interconnect networks with variable imperfect contact resistances. The MWCNT networks are represented using lumped RLGC MCC, hybrid, and ESC models in SPICE [32] while all other PC related computations are performed in MATLAB 2019a. In all the examples, the number of terms in the first-level and second-level corrector functions (i.e.,  $\bar{Q} + 1$  and  $R + 1$ , respectively) are controlled by the hyperbolic factors ( $u_1, u_2$ ) [10]. These hyperbolic factors are tuned such that the recovered PC metamodel of (14) exhibits an  $L_2$  error norm of  $10^{-3}$  or less (point of diminishing returns) with respect to the recovered PC metamodel trained by using previous value of the hyperbolic factor.

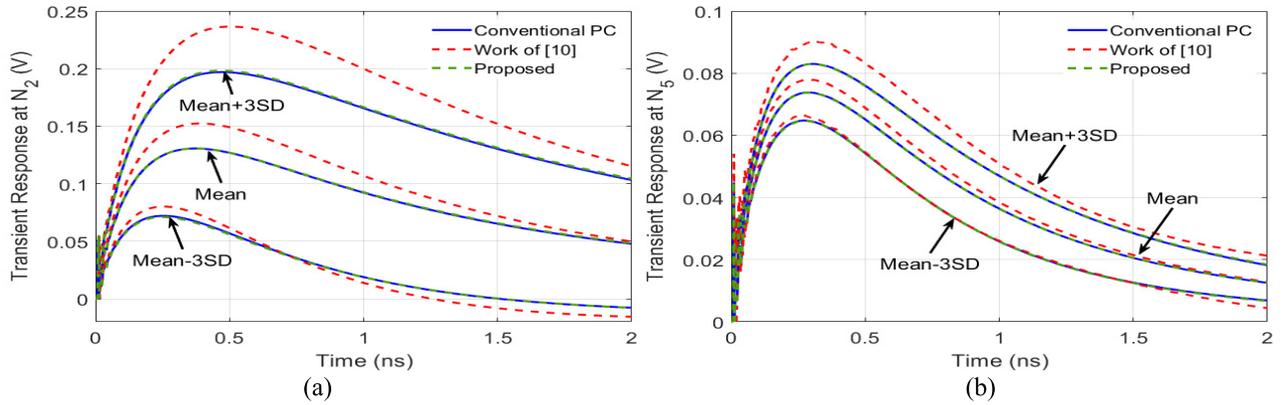
*Example 1* - In this example, a three ( $N_c = 3$ ) conductor MWCNT interconnect network as shown in Fig. 1 is considered. Each conductor has  $N_s = 30$  shells. The inner twenty shells of each conductor are perfectly contacted while the outer ten shells have imperfect contact resistances of 500 k $\Omega$ . Conductor 1 is excited using a voltage source with a saturated ramp waveform of rise time  $T_r = 0.1$  ps and amplitude 1 V. Conductors 2 and 3 are quiet. The response of interest for this example is the far-end transient response at node  $N_2$  of Fig. 1. There is a total of  $N = 15$  uncertain parameters in this example as listed in Table 1.

In order to perform UQ for this example, four PC metamodels are adopted – one trained using the single level multi-fidelity algorithm of [10] where the low-fidelity model is the ESC model, one trained using the single level multi-fidelity algorithm of [12] where the low-fidelity model is the hybrid model, the hyperbolic PC expansion approach of [22], and finally, the conventional PC metamodel trained using MCC model simulations. From [8], [9], [10], [11], it is clear that conventional PC captures the transient responses of MWCNT interconnect network accurately with much less computational burden as compared to Monte Carlo method which usually requires anywhere between 20,000 and 40,000 SPICE simulations to capture the responses accurately. Therefore, it is more convenient to compare the proposed approach against the conventional PC.

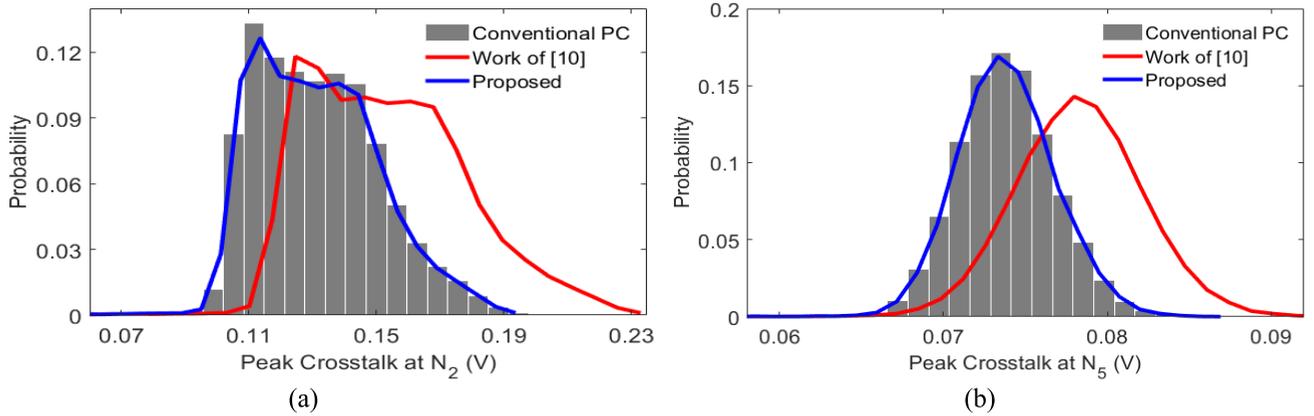
All PC metamodels require a maximum order of expansion  $m = 4$ . The number of terms used in the corrector for both multi-fidelity algorithms is set via the iterative hyperbolic PC expansion (HPCE) approach of [10] where the hyperbolic factor  $u = 0.8$ . The reason this specific value of the hyperbolic factor is chosen is because it is the highest possible value smaller than the limit  $u = 1$ . In effect, for  $u = 0.8$ , the recovered multi-fidelity PC metamodels will have the maximum possible accuracy without becoming identical to the conventional PC metamodel. Next, the statistics of the transient responses at node  $N_2$  is quantified using the aforementioned metamodels and their results are compared in Fig. 5(a). From Fig. 5(a), it is clearly observed that even for the maximum number of terms in the corrector function, the PC metamodel trained via the single level multi-fidelity algorithm of [10] displays significant errors in the standard deviation (SD) results. At this point, it is worth mentioning that the methodology of [10] and first level of [11] are the same. This implies that the work of [11] will have worse errors than [10] because it prunes unimportant dimensions from the PC expansion. On the other hand, the PC metamodel trained using the single level multi-fidelity algorithm of [12] leads to very accurate results. This difference in accuracy arises because of the more correct treatment of the imperfect contact resistances of the MWCNT shells in the hybrid model as opposed to the ESC model and is clearly quantified in Table 2. Moreover, this difference in the accuracy is even more distinct in the PDF estimate of the maximum crosstalk voltage at node  $N_2$  shown in Fig. 5(b). In all these comparisons, the hyperbolic PC metamodel of [22] is the most inaccurate.

At this juncture, it is pointed out that although the PC metamodel trained by the single level multi-fidelity algorithm of [12] is more accurate, this higher accuracy comes at the expense of the higher time cost to train the predictor. Indeed, the time cost to train the predictor using  $2(P + 1) = 6120$  SPICE hybrid model simulations is 1.03 hours compared to the 9.18 minutes required if the ESC model is used. In order to mitigate this higher training cost of the predictor, a PC metamodel of the network trained using the proposed bilevel multi-fidelity algorithm of Section III is also developed. In the proposed algorithm, the optimal number of terms in the first-level and second-level corrector metamodels of (10) and (13) respectively are determined using the iterative HPCE approach of [10] and these values correspond to the hyperbolic factors of  $(u_1, u_2) = (0.8, 0.5)$ . The response statistics and PDF of the maximum crosstalk at node  $N_2$  obtained using this method is shown in Fig. 6. It is observed from Fig. 6 that the results obtained from the proposed bilevel multi-fidelity algorithm shows good agreement with that from the conventional PC metamodel.

Table 2 compares the computational expense incurred in training the aforementioned PC metamodels where the time cost of a single ESC simulation ( $C_1$ ) = 0.09 seconds, that of a single hybrid simulation ( $C_2$ ) = 0.61 seconds, and that of a single MCC simulation ( $C_3$ ) = 8.29 seconds. Moreover,



**FIGURE 7.** Statistics of the transient responses of Example 2 computed using the PC metamodel trained by the single level multi-fidelity algorithm of [10], the proposed bilevel multi-fidelity algorithm, and the conventional PC metamodel. (a) Mean, mean plus three times the SD, and mean minus three times the SD of the transient response at node  $N_2$ . (b) Mean, mean plus three times the SD, and mean minus three times the SD of the transient response at node  $N_5$ .



**FIGURE 8.** PDF of the transient responses of Example 2 computed using the PC metamodel trained by the single level multi-fidelity algorithm of [10], the proposed bilevel multi-fidelity algorithm, and the conventional PC metamodel. (a) PDF of the peak crosstalk at node  $N_2$ . (b) PDF of the peak crosstalk at node  $N_5$ .

**TABLE 4.** Computational time cost for numerical example 2.

	# ESC model simulations	# Hybrid ESC-MCC model simulations	# MCC model simulations	CPU time cost	$L_2$ error norm of SD at node $N_2$ w. r. t. conventional PC	$L_2$ error norm of SD at node $N_5$ w. r. t. conventional PC	Speedup w. r. t. conventional PC
Conventional PC	0	0	10626	76 hours 38 minutes	-	-	-
Single level multi-fidelity algorithm of [10] ( $u = 0.8$ )	10626	0	1791	13 hours 43 minutes	0.189	0.115	5.59
Single level multi-fidelity algorithm of [12] ( $u = 0.7$ )	0	10626	651	12 hours 24 minutes	0.010	0.012	6.18
Reduced dimensional PC of [18]	0	0	1365	10 hours 43 minutes	0.011	0.016	7.78
Proposed bilevel multi-fidelity algorithm with $(u_1, u_2) = (0.7, 0.7)$	10626	651	651	5 hours 58 minutes	0.008	0.009	12.86

the number of ESC, hybrid, and MCC model simulations required to train each PC metamodel is also listed in Table 2.

In addition, in Table 2, the computational expense incurred by the non-multi-fidelity dimension reduction strategy of [18]

is also included for thoroughness of comparison. From the results of Table 2, it is observed that the proposed bilevel multi-fidelity algorithm is able to offer almost 5 times higher speedup than the single level multi-fidelity algorithm of [12]. Moreover, the proposed bilevel multi-fidelity algorithm also provides the best possible accuracy among all candidate methods including [12]. The speedup values of Table 2 are within the bounds specified in (19) and (20). Remarkably, the proposed bilevel multi-fidelity algorithm outperforms all the metamodels listed in Table 2, whether of the multi-fidelity variety or otherwise.

*Example 2* - In this example, a five ( $N_c = 5$ ) conductor MWCNT interconnect network as shown in Fig. 1 is considered. Each conductor has  $N_S = 50$  shells. The inner twenty shells of each conductor are perfectly contacted, the next ten shells have imperfect contact resistance of 100 k $\Omega$ , the next ten shells after that have imperfect contact resistance of 200 k $\Omega$ , and the outer ten shells have imperfect contact resistance of 500 k $\Omega$ . Conductor 1 and 3 are excited using a voltage source with a saturated ramp waveform of rise time  $T_r = 0.1$  ps and amplitude 1 V. Conductors 2, 4, and 5 are quiet. The responses of interest for this example are the far-end transient response for node  $N_1$ - $N_5$  of Fig. 1. There is a total of  $N = 20$  uncertain parameters in this example as listed in Table 3.

In order to perform UQ for this example, five PC metamodels are adopted – one trained using the proposed bilevel multi-fidelity algorithm described in Section III, one trained using the single level multi-fidelity algorithm of [10] where the low-fidelity model is the ESC model, one trained using the single level multi-fidelity algorithm of [12] where the low-fidelity model is the hybrid model, the hyperbolic PC metamodel of [22], and finally, the conventional PC metamodel trained only using MCC model simulations. All PC metamodels require a maximum order of expansion  $m = 4$ . The PC metamodels trained using the single level multi-fidelity algorithms of [10] and [12] uses optimal hyperbolic factors of  $u = 0.8$  and  $u = 0.7$  respectively. The PC metamodel trained using the proposed bilevel multi-fidelity algorithm uses the optimal hyperbolic factors of  $(u_1, u_2) = (0.7, 0.7)$ .

In the first part of this example, the statistics of the transient responses at nodes  $N_2$  and  $N_5$  are quantified using the aforementioned metamodels and their results are compared in Fig. 7. From Fig. 7, it is observed that the PC metamodel trained using the single level multi-fidelity algorithm of [10] is clearly unable to offer good accuracy despite using the maximum possible value of the hyperbolic factor  $u = 0.8$ . In contrast, the results obtained from the proposed bilevel multi-fidelity algorithm show good agreement with those obtained from the conventional PC metamodel despite using a lower  $u = 0.7$  (i.e., using a smaller number of terms). This difference in the accuracy of the two metamodels is also visible in the PDF estimate of the maximum crosstalk voltage at nodes  $N_2$  and  $N_5$  as shown in Fig. 8.

In the next stage of this example, the computational time costs incurred in training the aforementioned PC metamodels

are listed in Table 4. The time cost of a single ESC simulation ( $C_1$ ) = 0.27 seconds, that of a single hybrid ESC-MCC simulation ( $C_2$ ) = 2.61 seconds, and that of a single MCC simulation ( $C_3$ ) = 25.96 seconds. In Table 4, the computational expense incurred by the non-multi-fidelity dimension reduction strategy of [18] is also included for completeness of comparison. It is observed from Table 4 that the proposed bilevel multi-fidelity algorithm is able to more than double the speedup achieved by the single level multi-fidelity algorithm of [12]. In fact, not only is the proposed bilevel algorithm far more numerically efficient but also much more accurate than all candidate methods of Table 4. The speedup values of Table 4 are also within the bounds specified in (19) and (20).

## V. CONCLUSION

In this paper, a new bilevel multi-fidelity algorithm to perform uncertainty quantification of multi-walled carbon nanotube interconnect networks subject to variable imperfect contact resistances is presented. This algorithm leverages a hybrid model of the MWCNT conductors that is more accurate than the ESC model and more efficient to simulate than the rigorous MCC model. Therefore, the results obtained from the proposed hybrid model is guaranteed to exhibit better correlation with the true statistical results (i.e., the results from the MCC model) than what is possible using the ESC model. In this paper, this improved correlation is intelligently exploited using a bilevel multi-fidelity algorithm to yield faster convergence, and consequently, even higher speed up in training PC metamodels than what is possible using all existing single level multi-fidelity algorithms. This work focuses on developing PC metamodels which are linear combinations of smooth polynomials. These metamodels therefore cannot capture highly nonlinear and discontinuous parametric uncertainties (e.g., those existing in the geometry of the nonlinear CMOS driver/loads) and signal integrity quantities that exhibit a non-smooth functionality with respect to interconnect and CMOS driver/load parameters. However, this opens up the possibility of applying machine learning based techniques to perform signal integrity analysis of MWCNT interconnect networks.

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