Variational Capacitance Extraction and Modeling Based on Orthogonal Polynomial Method

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***Abstract*—In this paper, we propose a novel statistical capacitance extraction method for interconnect conductors considering process variations. The new method is called *statCap*, where orthogonal polynomials are used to represent the statistical processes in a deterministic way. We first show how the variational potential coefficient matrix is represented in a first-order form using Taylor expansion and orthogonal decomposition. Then, an augmented potential coefficient matrix, which consists of the coefficients of the polynomials, is derived. After this, corresponding augmented system is solved to obtain the variational capacitance values in the orthogonal polynomial form. Finally, we present a method to extend *statCap* to the second-order form to give more accurate results without loss of efficiency compared to the linear models. We show the derivation of the analytic second-order orthogonal polynomials for the variational capacitance integral equations. Experimental results show that *statCap* is two orders of magnitude faster than the recently proposed statistical capacitance extraction method based on the spectral stochastic collocation approach and many orders of magnitude faster than the Monte Carlo method for several practical conductor structures.**

***Index Terms*—Capacitance extraction, orthogonal decomposition, orthogonal polynomial, process variations.**

I. Introduction

IT IS WELL ACCEPTED that the process-induced variability has huge impacts on the circuit performance in the sub-100 nm VLSI technologies [14], [15]. The variational consideration of the process has to be assessed in various VLSI design steps to ensure robust circuit design. Process variations consist of both systematic ones, which depend on patterns and other process parameters, and random ones, which have to be dealt with using stochastic approaches. Efficient capacitance extraction approaches by using the boundary element method (BEM) such as the fastCap [12], HiCap [18], and PHiCap [22] have been proposed in the past. To consider the variation impacts on the interconnects, one has to consider the *RLC* extraction processes of the 3-D structures modeling the interconnect conductors. In this paper, we investigate the geometry variational impacts on the extracted capacitance.

Statistical extraction of capacitance considering process variations has been studied recently, and several approaches have been proposed [5],[8],[24]–[26] under different variational models. Method in [8] uses analytical formulae to consider the variations in capacitance extraction, and it has only first-order accuracy. The FastSies program considers the rough surface effects of the interconnect conductors[26]. It assumes only Gaussian distributions and has high computational costs. Method in [5] combines the hierarchical extraction and principle factor analysis to solve the capacitance statistical extraction.

Recently, a spectral stochastic-collocation-based capacitance extraction method was proposed [23] and [25]. This approach is based on the Hermite orthogonal polynomial representation of the variational capacitance. It applies the numerical quadrature (collocation) method to compute the coefficients of the extracted capacitances in the Hermite polynomial form where the capacitance extraction processes (by solving the potential coefficient matrices) are performed many times (sampling). One of the major problems with this method is that many redundant operations are carried out (such as the setup of potential coefficient matrices for each sampling, which corresponds to solve one particular extraction problem). For the second-order Hermite polynomials, the number of samplings is $\mathrm{O}(m^2)$, where m is the number of variables. Therefore, if m is large, the approach will lose its efficiency compared to the Monte Carlo (MC) method.

In this paper, instead of using the numerical quadrature method, we use a different spectral stochastic method, where the Galerkin scheme is used. Galerkin-based spectral stochastic method has been applied for statistical interconnect modeling [2], [19] and on-chip power grid analysis considering process variations in the past [9]–[11]. The new method, called *statCap*, first transforms the original stochastic potential coefficient equations into a deterministic and larger one (via the Galerkin method), and then, solves it using an iterative method. It avoids the less-efficient sampling process in the existing collocation-based extraction approach. As a result, the potential coefficient equations and the corresponding augmented system need to be set up only once versus many times in the collocation-based sampling method. This can lead to a significant saving in CPU time. Also, the augmented potential coefficient system is sparse, symmetric, and low rank, which is further exploited by an iterative solver to gain further speedup.

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To consider second-order effects, we derive the closed-form orthogonal polynomials for the capacitance integral equations directly in terms of variational variables without the loss of speed compared with the linear model. Experimental results show that the proposed method based on the first-order and second-order effects can deliver two orders of magnitude speedup over the collocation-based spectral stochastic method and many orders of magnitude over the MC method.

The main contributions of the this paper are as follows.

1) The Galerkin-based spectral stochastic method is proposed to solve the statistical capacitance extraction problem where Galerkin scheme (versus the collocation method) is used to compute the coefficients of capacitances.
2) The closed-form coefficients hermite polynomial is derived for potential coefficient matrices in both first-order and second-order forms.
3) The augmented matrix properties are studied, showing that augmented matrix is still quite sparse, low rank, and symmetric.
4) The augmented systems are solved by minimum-residue conjugate gradient method [16] to take advantage of the sparsity, low rank, and symmetric properties of the augmented matrices.
5) The method is compared with the existing statistical capacitance extraction method based on the spectral stochastic collocation approach [25] and MC method, showing the superiority of the proposed method.

We remark that we have put less emphasis on the acceleration techniques during the extraction processes, such as the multiple-pole scheme [12]and the hierarchical methods [18], [22], using the more sophisticated iterative solvers such as general minimal residue (GMRES) [17], which actually are the key components of these methods. The reason is that this is not the focus area where our major contributions are made. We believe that these existing acceleration techniques can significantly speedup the proposed method as they did for the deterministic problem. This is especially the case for the hierarchical approach [18], where the number of panels (thus, the random variables) can be considerably reduced and the interaction between panels are constant. These are the areas for our future investigations.

The rest of this paper is organized as follows. Section II presents statistical capacitance extraction problem to be solved. Section III reviews the orthogonal-polynomial-chaos (PC) based stochastic simulation methods. Section IV presents our new statistical capacitance extraction method considering first-order perturbations. Then, Section V presents the new method considering the second-order effects. Section VI presents the experimental results and Section VII concludes this paper.

II. Problem Formulation

For m conductors system, the capacitance extraction problem based on the BEM formulation is to solve the following integral equation [12]:

$$\int_S \frac{1}{|\vec{x}_i - \vec{x}_j|}\rho(\vec{x}_j)da_j = v(\vec{x}_i) \tag{1}$$

where $\rho(\vec{x}_j)$ is the charge distribution on the surface at conductor j, $v(\vec{x}_i)$ is the potential at conductor i, $1/|\vec{x}_i - \vec{x}_j|$ is the free-space Green function,[1] da_j is the surface area on the surface S of conductor j, and $\vec{x}_i$ and $\vec{x}_j$ are point vectors. To solve for capacitances from one conductor to the rest of others, we set the conductor's potential to be 1 and all other $m-1$ conductors' potential to be 0. The resulting charges that are computed are capacitances. BEM method divides the surfaces into N small panels and assume uniform charge distribution on each panel, which transforms (1) into a linear algebraic equation

$$Pq = v \tag{2}$$

where $P \in R^{N\times N}$ is the potential coefficient matrix, q is the charge on panels, v is the preset potential on each panel. By solving the aforementioned linear equation, we can obtain all the panel charges (thus, capacitance values). In potential coefficient matrix P, each element is defined as

$$P_{ij} = \frac{1}{s_j}\int_{S_j} G(\vec{x}_i, \vec{x}_j)da_j \tag{3}$$

where $G(\vec{x}_i, \vec{x}_j) = 1/|\vec{x}_i - \vec{x}_j|$ is the Green function of point source at $\vec{x}_j$, S_j is the surface of panel j, and s_j is the area of panel j.

Process variations introducing conductor geometry variations are reflected on the fact that the size of the panel and distances between panels become random variables. Here, we assume that the panel is still a 2-D surface. These variations will make each element in capacitance matrix follow some kinds of random distributions. The problem that we need to solve now is to derive this random distribution, and then to effectively compute the mean and variance of involved capacitance given the geometry randomness parameters.

In this paper, we follow the variational model introduced in [5], where each point in panel i is disturbed by a vector Δn_i that has the same direction as the normal direction of panel i

$$\vec{x}_i' = \vec{x}_i + \Delta n_i \tag{4}$$

where the length of the Δn_i follows Gaussian distribution $|\Delta n_i| \sim N(0, \sigma^2)$. If the value is negative, it means that the direction of the perturbation is reversed. The correlation between random perturbation on each panel is governed by the empirical formulation such as the exponential model [26]

$$\gamma(r) = e^{-r^2/\eta^2} \tag{5}$$

where r is the distance between two panel centers and η is the correlation length.

The most straightforward method is to use MC simulation to obtain distributions, mean values, and variances of all these capacitances. But the MC method will be extremely time-consuming as each sample run requires the formulation of the changed potential coefficient matrix P.

[1]Note that the scale factor $1/(4\pi\epsilon_0)$ can be ignored here to simplify the notation and is used in the implementation to give results in units of farads.

III. Review of Spectral Stochastic Method

In this section, we briefly review the spectral stochastic or orthogonal PC-based stochastic analysis methods.

A. Concept of Hermite PC

In the following, a random variable $\xi(\theta)$ is expressed as a function of θ, which is the random event. Hermite PC utilizes a series of orthogonal polynomials (with respect to the Gaussian distribution) to facilitate stochastic analysis [4], [21]. These polynomials are used as orthogonal basis to decompose a random process.

We remark that for the Gaussian and log-normal distributions, using Hermite polynomials is the best choice as they lead to exponential convergence rate [4]. For non-Gaussian and nonlog-normal distributions, there are other orthogonal polynomials such as Legendre for uniform distribution, Charlier for Poisson distribution, Krawtchouk for Binomial distribution, etc. [3], [19].

Given a random variable $v(t,\xi)$ with variation, where $\xi = [\xi_1,\ldots,\xi_n]$ denotes a vector of orthonormal Gaussian random variables with zero mean, the random variable can be approximated by a truncated Hermite PC expansion as follows [4]:

$$v(t,\xi) = \sum_{k=0}^{P} a_k H_k^n(\xi) \tag{6}$$

where n is the number of independent random variables, $H_k^n(\xi)$ are n-dimensional Hermite polynomials, and a_k are the deterministic coefficients. The number of terms P is given by

$$P = \sum_{k=0}^{p} \frac{(n-1+k)!}{k!(n-1)!} \tag{7}$$

where p is the order of the Hermite PC. For simplification of explanation, only one random variable is considered, and the 1-D Hermite polynomials are expressed as follows:

$$\begin{aligned} H_0^1(\xi) &= 1, \qquad H_1^1(\xi) = \xi, \\ H_2^1(\xi) &= \xi^2 - 1, \qquad H_3^1(\xi) = \xi^3 - 3\xi, \ldots. \end{aligned} \tag{8}$$

The Hermite polynomials are orthogonal with respect to Gaussian weighted expectation (the superscript n is dropped for simple notation)

$$\langle H_i(\xi), H_j(\xi)\rangle = \langle H_i^2(\xi)\rangle \delta_{ij} \tag{9}$$

where δ_{ij} is the Kronecker delta and $\langle *, *\rangle$ denotes an inner product defined as

$$\langle f(\xi), g(\xi)\rangle = \frac{1}{\sqrt{(2\pi)^n}} \int f(\xi) g(\xi) e^{-1/2\xi^T \xi} d\xi. \tag{10}$$

Thus, the coefficients a_k are evaluated by the projection operation onto the Hermite PC basis

$$a_k(t) = \frac{\langle v(t,\xi), H_k(\xi)\rangle}{\langle H_k^2(\xi)\rangle} \qquad \forall k \in \{0,\ldots,P\}. \tag{11}$$

B. Computing Coefficients, the Mean and Variance From Hermite PCs

In case that $q(\xi)$ in (2) is unknown random variable vector (with normal distribution), then potential coefficient equation become

$$P(\xi) q(\xi) = v \tag{12}$$

where both $P(\xi)$ and $q(\xi)$ are in Hermite PC form. Then, the coefficients can be computed by using Galerkin method. The principle of orthogonality states that the best approximation of $v(\xi)$ is obtained when the error $\Delta(\xi)$ defined as

$$\Delta(\xi) = P(\xi) q(\xi) - v \tag{13}$$

is orthogonal to the approximation, i.e.

$$\langle \Delta(\xi), H_k(\xi)\rangle = 0, \qquad k = 0, 1, \ldots, P \tag{14}$$

where $H_k(\xi)$ are Hermite polynomials. In this way, we have transformed the stochastic analysis process into a deterministic form, whereas we only need to compute the corresponding coefficients of the Hermite PC.

For the illustration purpose, considering two Gaussian variable $\xi = [\xi_1, \xi_2]$, we assume that the charge vector in panels can be written as a second-order $(p = 2)$ Hermite PC, we have

$$q(\xi) = q_0 + q_1\xi_1 + q_2\xi_2 + q_3(\xi_1^2 - 1) + q_4(\xi_2^2 - 1) + q_5(\xi_1\xi_2) \tag{15}$$

which will be solved by using augmented potential coefficient matrices to be discussed in Section IV. Once the Hermite PC of $q(\xi)$ is known, the mean and variance of $q(\xi)$ can be evaluated trivially. Given an example, for one random variable, the mean and variance are calculated as

$$\begin{aligned} E(q(\xi)) &= q_0 \\ \mathrm{Var}(q(\xi)) &= q_1^2 \mathrm{Var}(\xi) + q_2^2 \mathrm{Var}(\xi^2 - 1) \\ &= q_1^2 + 2q_2^2. \end{aligned} \tag{16}$$

In consideration of correlations among random variables, we apply principal component analysis (PCA) to transform the correlated variables into a set of independent variables.

IV. New Orthogonal-Polynomial-Based Extraction Method: statCap

In this section, we present our new spectral stochastic-method-based method, *statCap*, which uses the orthogonal polynomials to represent random variables starting from the geometry parameters.

In our new method, we first represent the variation potential matrix P into a first-order form using Taylor expansion. We then extend our method to handle the second-order variations in Section V.

A. Expansion of Potential Coefficient Matrix

Specifically, each element in the potential coefficient matrix P can be expressed as

$$P_{ij} = \frac{1}{s_j \int_{S_j} G(\vec{x}_i, \vec{x}_j) da_j} \tag{17}$$

where $G(\vec{x}_i, \vec{x}_j)$ is the free-space Green function defined in (3).

Note that if panels i and j are far away (their distance is much larger than the panel area), we can have the following approximation [5]:

$$P_{ij} \approx G(\vec{x}_i,\ \vec{x}_j), \qquad i \neq j. \tag{18}$$

Suppose variation of panel i can be written as $\Delta n_i = \delta i \vec{n}_i$, where $\vec{n}_i$ is the unit normal vector of panel i and δi is the scalar variation. Then, take Taylor expansion on the Green function as

$$G(\vec{x}_i + \Delta n_i, \vec{x}_j + \Delta n_j) = \frac{1}{|\vec{x}_i - \vec{x}_j + \Delta n_i - \Delta n_j|} \tag{19}$$

$$= \frac{1}{|\vec{x}_i - \vec{x}_j|} + \nabla \frac{1}{|\vec{x}_i - \vec{x}_j|} \cdot (\Delta n_j - \Delta n_i) + O((\Delta n_i - \Delta n_j)^2). \tag{20}$$

From free-space Green function, we have

$$\nabla G(\vec{x}_i, \vec{x}_j) = \nabla \frac{1}{|\vec{x}_i - \vec{x}_j|} = \nabla \frac{1}{|\vec{r}|} = \frac{\vec{r}}{|\vec{r}|^3} \tag{21}$$

$$\vec{r} = \vec{x}_i - \vec{x}_j. \tag{22}$$

Now, we first ignore the second-order terms to make the variation in the linear form. As a result, the potential coefficient matrix P can be written as (23), which is shown at the bottom of the page. We can further write P_1 as (24), which is shown at the bottom of the next page, where J_1 and N_1 are vector matrices, and V_1 is the diagonal matrix.

To deal with spatial correlation, P_1 can be further expressed as a linear combination of the dominate and independent variables

$$\xi = [\xi_1, \xi_2, \ldots, \xi_p] \tag{25}$$

through the PCA operation. As a result, V_1 can be further expressed as

$$\begin{pmatrix} \sum_{i=1}^{p} a_{1i}\xi_i & 0 & \cdots \\ 0 & \sum_{i=1}^{p} a_{2i}\xi_i & \cdots \\ \vdots & \cdots & \vdots \\ \cdots & 0 & \sum_{i=1}^{p} a_{ni}\xi_i \end{pmatrix}. \tag{26}$$

Finally, we can represent P_1 as

$$P_1 = \sum P_{1i}\xi_i \tag{27}$$

where

$$P_{1i} = A_i N_1 J_1 - J_1 N_1 A_i \tag{28}$$

and

$$A_i = \begin{pmatrix} a_{1i} & 0 & \ldots & 0 \\ 0 & a_{2i} & \ldots & 0 \\ \vdots & \vdots & \ldots & \vdots \\ 0 & \ldots & 0 & a_{ni} \end{pmatrix}. \tag{29}$$

B. Formulation of the Augmented System

Once the potential coefficient matrix is represented in the affine form, as shown in (27), we are ready to solve for the coef-

$$P \approx P_0 + P_1 = \begin{pmatrix} G(\vec{x}_1 + \Delta n_1, \vec{x}_1 + \Delta n_1) & \ldots & G(\vec{x}_1 + \Delta n_1, \vec{x}_n \Delta n_n) \\ G(\vec{x}_2 + \Delta n_2, \vec{x}_1 + \Delta n_1) & \ldots & G(\vec{x}_2 + \Delta n_2, \vec{x}_n \Delta n_n) \\ \vdots & \ldots & \vdots \\ G(\vec{x}_n + \Delta n_n, \vec{x}_1 + \Delta n_1) & \ldots & G(\vec{x}_n + \Delta n_n, \vec{x}_n \Delta n_n) \end{pmatrix} \tag{23}$$

$$P_0 = \begin{pmatrix} G(\vec{x}_1, \vec{x}_1) & G(\vec{x}_1, \vec{x}_2) & \ldots & G(\vec{x}_1, \vec{x}_n) \\ G(\vec{x}_2 \vec{x}_1) & G(\vec{x}_2, \vec{x}_2) & \ldots & G(\vec{x}_2, \vec{x}_n) \\ \vdots & \vdots & \ldots & \vdots \\ G(\vec{x}_n, \vec{x}_1) & G(\vec{x}_n, \vec{x}_2) & \ldots & G(\vec{x}_n, \vec{x}_n) \end{pmatrix}$$

$$P_1 = \begin{pmatrix} 0 & \ldots & \nabla G(\vec{x}_1, \vec{x}_n)(\Delta n_n - \Delta n_1) \\ \nabla G(\vec{x}_2, \vec{x}_1)(\Delta n_1 - \Delta n_2) & \ldots & \nabla G(\vec{x}_2, \vec{x}_n)(\Delta n_n - \Delta n_2) \\ \vdots & \ldots & \vdots \\ \nabla G(\vec{x}_n, \vec{x}_1)(\Delta n_1 - \Delta n_n) & \ldots & 0 \end{pmatrix}.$$

ficients P_{1i} by using the Galerkin method, which will result in a larger system with augmented matrices and variables.

Specifically, for p-independent Gaussian random variables $\xi = [\xi_1, \ldots, \xi_p]$, there are $K = 2p + p(p-1)/2$ first- and second-order Hermite polynomials. $H_i(\xi)\ i = 1, \ldots, K$ represents each Hermite polynomial and $H_1 = \xi_1, \ldots, H_p = \xi_p$. Therefore, for the vector of variational potential variables $q(\xi)$, it can be written as

$$q(\xi) = q_0 + \sum_{i=1}^{K} q_i H_i(\xi) \tag{30}$$

where each q_i is a vector associated with one polynomial. So, the random linear equation can be written as

$$Pq = \left(P_0 + \sum_{i=1}^{p} P_{1i} H_i\right)\left(q_0 + \sum_{i=1}^{K} q_i H_i\right) = v. \tag{31}$$

Expanding the equation and performing inner product with H_i on both sides, we can derive new linear system equations

$$\left(W_0 \otimes P_0 + \sum_{i=1}^{p} W_i \otimes P_{1i}\right) Q = V \tag{32}$$

where $\otimes$ is the tensor product and

$$Q = \begin{pmatrix} q_0 \\ q_1 \\ \vdots \\ q_K \end{pmatrix} \qquad V = \begin{pmatrix} v \\ 0 \\ \vdots \\ 0 \end{pmatrix} \tag{33}$$

and see (34) at the bottom of the page, where $\langle H_i H_l H_m \rangle$ represents the inner product of three Hermite polynomial H_i, H_l, and H_m. The matrix $(W_0 \otimes P_0 + \sum_{i=1}^{p} W_i \otimes P_{1i})$ in (32) is called the *augmented potential coefficient* matrix. Since H_i are at most second-order polynomials, we can quickly calculate every element in W_i with a lookup table for any number of random variables.

We remark that matrices W_i are very sparse due to the nature of the inner product. As a result, their tensor products with P_{1i} will also lead to the very sparse augmented matrix in (32). As a result, we have the following observations regarding the structure of the W_i and the augmented matrix.

1) *Observation 1:* W_0 is a diagonal matrix.
2) *Observation 2:* For W_i matrices, $i \neq 0$, all the diagonal elements are zero.
3) *Observation 3:* All W_i are symmetric and the resulting augmented matrix $W_0 \otimes P_0 + \sum_{i=1}^{p} W_i \otimes P_{1i}$ is also symmetric.
4) *Observation 4:* If one element at position (l, m) in W_i is not zero, i.e., $W_i(l, m) \neq 0$, then elements at the same position (l, m) of $W_j, j \neq i$, must be zero. In other words

$$W_i(l,m) p W_j(l,m) = 0, \qquad \text{when } i \neq j \quad \forall\, i, j = 1, \ldots, p \text{ and } l, m = 1, \ldots, K.$$

Such sparse property can help save the memory significantly as we do not need to actually perform the tensor product, as shown in (32). Instead, we can add all W_i together and expand each element in the resulting matrix by some specific P_{1i} during the solving process, as there is no overlap among W_i for any element position.

As the original potential coefficient matrix is quite sparse and low rank, the augmented matrix is also low rank. As a result, the sparsity, low rank, and symmetric properties can be exploited by iterative solvers to speed up the extraction process, as shown in

$$\begin{aligned}
P_1 &= V_1 N_1 J_1 - J_1 N_1 V_1 \\
J_1 &= \begin{pmatrix} 0 & \nabla G(\vec{x}_1, \vec{x}_2) & \ldots & \nabla G(\vec{x}_1, \vec{x}_n) \\ \nabla G(\vec{x}_2, \vec{x}_1) & 0 & \ldots & \nabla G(\vec{x}_2, \vec{x}_n) \\ \vdots & \vdots & \ldots & \vdots \\ \nabla G(\vec{x}_n, \vec{x}_1) & \ldots & \nabla G(\vec{x}_n, \vec{x}_{n-1}) & 0 \end{pmatrix} \\
N_1 &= \begin{pmatrix} \vec{n}_1 & 0 & \ldots \\ 0 & \vec{n}_2 & \ldots \\ \vdots & \ldots & \vdots \\ 0 & \ldots & \vec{n}_n \end{pmatrix} \\
V_1 &= \begin{pmatrix} \delta n_1 & 0 & \ldots \\ 0 & \delta n_2 & \ldots \\ \vdots & \ldots & \vdots \\ 0 & \ldots & \delta n_n \end{pmatrix}
\end{aligned} \tag{24}$$

$$W_i = \begin{pmatrix} \langle H_i H_0 H_0 \rangle & \langle H_i H_0 H_1 \rangle & \ldots & \langle H_i H_0 H_K \rangle \\ \langle H_i H_1 H_0 \rangle & \langle H_i H_1 H_1 \rangle & \ldots & \langle H_i H_1 H_K \rangle \\ \vdots & \vdots & \langle H_i H_l H_m \rangle & \vdots \\ \langle H_i H_K H_0 \rangle & \langle H_i H_K H_1 \rangle & \ldots & \langle H_i H_K H_K \rangle \end{pmatrix} \tag{34}$$

the experimental results. In our implementation, the minimum residue conjugate gradient method [16] is used as the solver since the augmented system is symmetric.

V. Second-Order *Statcap*

In this section, we extend *StatCap* to consider second-order perturbations. We show the derivation of the coefficient matrix element in second-order orthogonal polynomial from the geometric variables. As a result, the second-order potential coefficient matrix can be computed very quickly. In our second-order *StatCap*, we consider both the far-field and near-field cases when (17) is approximated.

A. Derivation of Analytic Second-Order Potential Coefficient Matrix

Each element in the potential coefficient matrix P can be expressed as

$$\begin{aligned} P_{ij} &= \frac{1}{s_i s_j}\int_{S_i}\int_{S_j} G(\vec{x}_i,\vec{x}_j)da_i da_j \\ &\approx \frac{1}{s_j}\int_{S_j} G(x_i,\vec{x}_j)da_j \qquad (35)\\ &\approx \frac{1}{s_i}\int_{S_i} G(x_i,\vec{x}_j)da_i \qquad (36)\end{aligned}$$

where $G(\vec{x}_i,\vec{x}_j)$ is the free-space Green function defined in (3).

We assume the same definitions for Δn_i, δn_i, and $\vec{n}_i$, as in Section IV. If we consider both first-order and second-order terms, we have the following Taylor expansion on P_{ij}

$$\begin{aligned} &P_{ij}(\Delta n_i,\Delta n_j)\\ &=P_{i,j,0}+\nabla P_{ij}\Delta n_i+\nabla P_{ij}\Delta n_j\\ &\quad+\Delta {n_j}^T\nabla^2 P_{ij}\Delta n_j+\Delta {n_i}^T\nabla^2 P_{ij}\Delta n_i\\ &\quad+2\Delta {n_j}^T\nabla^2 P_{ij}\Delta n_i+O((\Delta n_i-\Delta n_j)^3)\\ &\approx P_{i,j0}+\frac{\partial P_{ij}}{\partial \Delta n_i}\delta n_i+\frac{\partial P_{ij}}{\partial \Delta n_j}\delta n_j\\ &\quad+\frac{\partial^2 P_{ij}}{\partial {\Delta n_i}^2}{\delta n_i}^2+\frac{\partial^2 P_{ij}}{\partial {\Delta n_j}^2}{\delta n_j}^2\\ &\quad+2\frac{\partial^2 P_{ij}}{\partial \Delta n_i \Delta n_j}\delta n_i\delta n_j. \qquad (37)\end{aligned}$$

And to deal with the spatial correlation, Δn_i can be further expressed as a linear combination of the dominate and independent variables in (25) through the PCA operation. As a result

$$\Delta n_i = \delta n_i \vec{n}_i = (a_{i1}\xi_1+\cdots+a_{ip}\xi_p)\vec{n}_i \qquad (38)$$

where a_{iL} is defined in (26). After this, P will be represented by a linear combination of Hermite polynomials

$$\begin{aligned} P = P_0+\sum_{L=1}^{p}P_{1L}\xi_L+\sum_{L=1}^{p}P_{2L}(\xi_L^2-1)\\ +\sum_{L_1}^{L_1\neq L_2}\sum_{L_2}P_{2L_1,L_2}\xi_{L_1}\xi_{L_2} \qquad (39)\end{aligned}$$

where P_{2L} is the coefficient corresponding to the first type of second-order Hermite polynomial, ξ_L^2-1, and P_{2L_1,L_2} means the coefficient corresponding to the second type of second-order Hermite polynomial, $\xi_{L_1}\xi_{L_2}(L_1\neq L_2)$.

Therefore, for each element P_{ij} in P, the coefficients of orthogonal polynomials can be computed as follows:

$$\begin{aligned} P_{ij,1L} &= a_{iL}\frac{\partial P_{ij}}{\partial \Delta n_i}+a_{jL}\frac{\partial P_{ij}}{\partial \Delta n_j} \qquad (40)\\ P_{ij,2L} &= a_{iL}^2\frac{\partial^2 P_{ij}}{\partial {\Delta n_i}^2}+a_{jL}^2\frac{\partial^2 P_{ij}}{\partial {\Delta n_j}^2}\\ &\quad+2a_{iL}a_{jL}\frac{\partial^2 P_{ij}}{\partial \Delta n_j \Delta n_i} \qquad (41)\\ P_{ij,2L_1,L_2} &= 2a_{iL_1}a_{iL_2}\frac{\partial^2 P_{ij}}{\partial {\Delta n_i}^2}+2a_{jL_1}a_{jL_2}\frac{\partial^2 P_{ij}}{\partial {\Delta n_j}^2}\\ &\quad+2(a_{iL_1}a_{jL_2}+a_{iL_2}a_{jL_1})\frac{\partial^2 P_{ij}}{\partial \Delta n_j \Delta n_i}. \qquad (42)\end{aligned}$$

Hence, we need to compute analytic expressions for the partial derivatives of P_{ij} to obtain the coefficients of Hermite polynomials. The details of the derivations for computing the derivatives used in (40), (42), and (42) can be found in the Appendix section.

B. Formulation of the Augmented System

Similarly, as in Section IV, once the potential coefficient matrix is represented in the affine form, as shown in (39), we are ready to solve the coefficients P_{1L}, P_{2L}, and P_{2L_1,L_2} by using the Galerkin method.

In this case, P in (39) is now rewritten as

$$P = P_0+\sum_{i=1}^{p}P_{1i}H_i+\sum_{i=p+1}^{K}P_{2i}H_i. \qquad (43)$$

So, after considering the first-order and second-order Hermite polynomials in P, the random linear equation can be written as

$$\begin{aligned} Pq = \left(P_0+\sum_{i=1}^{p}P_{1i}H_i+\sum_{i=p+1}^{K}P_{2i}H_i\right)\\ \cdot\left(q_0+\sum_{i=1}^{K}q_iH_i\right)=v. \qquad (44)\end{aligned}$$

Expanding the equation and performing inner product with H_i on both sides, we can derive a new linear system as

$$\left(W_0\otimes P_0+\sum_{i=1}^{p}W_i\otimes P_{1i}+\sum_{i=p+1}^{K}W_i\otimes P_{2i}\right)Q=V \qquad (45)$$

where $\otimes$ is the tensor product, Q and V are same as in (33), and W_i has the same definition as in (34).

Again, the matrix in the right-hand side of (45) is the *augmented potential coefficient* matrix for the second-order *statCap*. Since H_i are at most second-order polynomials, we can still use lookup table to calculate every element in W_i for any number of random variables.

Now, we study the properties of augmented potential coefficient matrix. We review the features and observations that we made for the first-order *statCap*.

TABLE I
NUMBER OF NONZERO ELEMENT IN W_i

	$i=0$	$1 \le i \le p$	$p+1 \le i \le 2p$	$2p+1 \le i \le K$
# non-zero	K	2p+2	p+3	2p+4

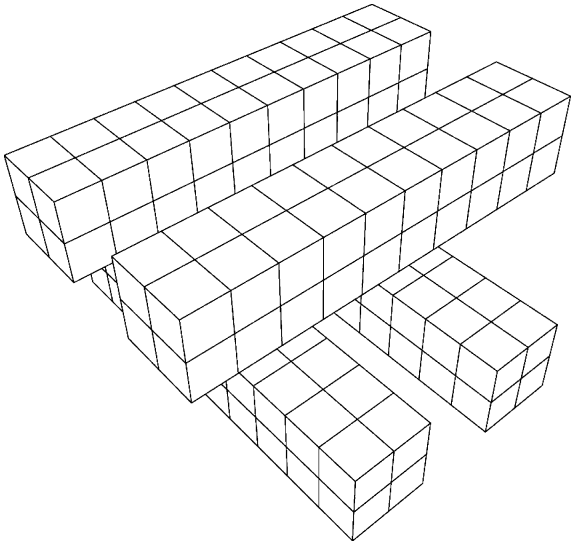

Fig. 1. 2×2 bus.

For W_i, which is a $K \times K$ matrix, where $K = p(p+3)/2$, the number of nonzero elements in W_i is showed in Table I. From Table I, we can see that matrices W_i for $i = 1, \ldots, K$ are still very sparse. As a result, their tensor products with P_{1i} and P_{2i} will still give rise to the sparse augmented matrix in (45).

For the four observations in Section IV regarding the structure of $W_i, where i = p+1, \ldots, K$, and the augmented matrix, we find that all the observations are still valid except for Observation 2. As a result, all the efficient implementation and solving techniques mentioned at the end of Section IV can be applied to the second-order method.

VI. EXPERIMENTAL RESULTS

In this section, we compare the results of the proposed first-order and second-order *statCap* methods against the MC method and the SSCM method [25], which is based on the spectral stochastic collocation method. The proposed *statCap* methods have been implemented in MATLAB 7.4.0. We use minimum residue conjugate gradient method as the iterative solver. We also implement the SSCM method in MATLAB using the sparse grid package [6], [7]. We do not use any hierarchical algorithm to accelerate the calculation of the potential coefficient matrix for both *statCap* and SSCM. Instead, we use analytic formula in [20] to compute the potential coefficient matrices.

All the experimental results are carried out in a Linux system with Intel Quadcore Xeon CPUs with 2.99 GHz and 16 GB memory.

We test our algorithm on six testing cases. The more specific running parameters for each testing cases are summarized in Table II. In Table II, p is the number of dominate and independent random variables that we get through PCA operation, and $MC\#$ means the times we run MC method. The 2×2 bus is shown in Fig. 1, and three-layer metal plane capacitance is shown in Fig. 2. In all the experiments, we set standard deviation as 10% of the wire width and the η, the correlation length, as 200% of the wire width.

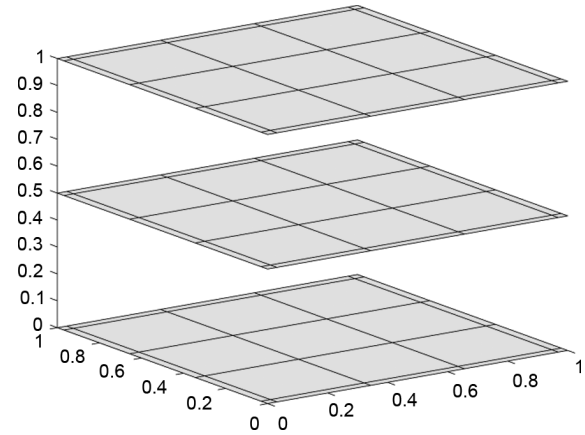

Fig. 2. Three-layer metal planes.

TABLE II
TEST CASES AND THE PARAMETERS SETTING

	1x1 bus	2x2 bus	3-layer	3x3 bus	4x4 bus	5x5 bus
Panel #	28	352	75	720	1216	4140
p	10	15	8	21	28	35
MC #	10000	6000	6000	6000	6000	6000

TABLE III
CPU RUNTIME (IN SECONDS) COMPARISON AMONG MC, SSCM, AND $statCap\ (First/Second)$

1×1 bus, MC(10000)					
MC	SSCM	*statCap(1st)*	*statCap(2nd)*	SP(MC)	SP(SSCM)
2764s	49.35s	1.55s	3.59s	1783	32
2×2 bus, MC(6000)					
MC	SSCM	*statCap(1st)*	*statCap(2nd)*	SP(MC)	SP(SSCM)
63059s	2315s	122s	190s	517	19
3-layer metal plane, MC(6000)					
MC	SSCM	*statCap(1st)*	*statCap(2nd)*	SP(MC)	SP(SSCM)
16437s	387s	4.11s	6.67s	3999	94
3×3 bus, MC(6000)					
MC	SSCM	*statCap(1st)*	*statCap(2nd)*	SP(MC)	SP(SSCM)
2.2×10^5s	7860s	408s	857s	534	19
4×4 bus, MC(6000)					
MC	SSCM	*statCap(1st)*	*statCap(2nd)*	SP(MC)	SP(SSCM)
–*	3.62×10^4	1573s	6855s	260	23
5×5 bus, MC(6000)					
MC	SSCM	*statCap(1st)*	*statCap(2nd)*	SP(MC)	SP(SSCM)
–*	–	1.7×10^4	6.0×10^4s	–	–

* – out of memory

First, we compare the CPU times of the four methods. The results are shown in Table III. In the table, *statCap(first/second)* refer to the proposed first- and second-order methods, respectively. $SP(X)$ means the speed up of the first-order *StatCap* comparing with MC or SSCM. All the capacitances are in picofarads.

It can be seen that both the first- and second-order *statCap* are much faster than both SSCM and the MC method. And for large testing cases, such as the 5×5 bus case, MC and SSCM will run out of memory, but *statCap* still work well. For all the cases, *statCap* can deliver about two orders of magnitude speedup over the SSCM and three orders of magnitude speedup

TABLE IV
CAPACITANCE MEAN VALUE COMPARISON FOR THE 1×1 BUS

	MC	SSCM	*statCap(1st)*	*statCap(2nd)*
C11	135.92	135.90	136.58	136.21
C12	-57.11	-57.01	-57.49	-57.27
C21	-57.11	-57.02	-57.49	-57.27
C22	135.94	135.69	136.58	136.21

TABLE V
CAPACITANCE STANDARD DEVIATION COMPARISON FOR THE 1×1 BUS

	MC	SSCM	*statCap(1st)*	*statCap(2nd)*
C11	2.42	2.49	3.13	2.63
C12	1.71	1.74	2.02	1.86
C21	1.72	1.71	2.02	1.86
C22	2.51	2.52	3.19	2.63

TABLE VI
ERROR COMPARISON OF CAPACITANCE MEAN VALUES AMONG SSCM AND $statCap$ (FIRST AND SECOND ORDER)

1×1 bus, MC(10000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	0.19%	0.67%	0.28%
Avg err	0.14%	0.57%	0.24%
2×2 bus, MC(6000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	0.32%	0.49%	1.19%
Avg err	0.15%	0.24%	0.89%
3-layer metal plane, MC(6000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	0.30%	1.84%	0.81%
Avg err	0.14%	0.90%	0.58%
3×3 bus, MC(6000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	0.33%	0.81%	0.43%
Avg err	0.11%	0.58%	0.11%
4×4 bus, SSCM as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	0	0.76%	0.35%
Avg err	0	0.40%	0.09%
5×5 bus, *StatCap(2nd)* as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	–	0.59%	0
Avg err	–	0.28%	0

over MC method. Note that both SSCM and *statCap* use the same random variables after PCA reduction.

We note that both MC and SSCM need to compute the potential coefficient matrices each time the geometry changes. This computation can be significant compared to the CPU time of solving potential coefficient equations. This is one of the reasons that SSCM and MC are much slower than *statCap*, in which the augmented system only needs to be setup once.

Also, SSCM uses the sparse grid scheme to reduce the collocation points in order to derive the orthogonal polynomial coefficients. But the number of collocation points are still in the order of $O(m^2)$ for the second-order Hermit polynomials, where m is the number of variables. Thus, it requires $O(m^2)$ solutions for the different geometries. In our algorithm, we also consider the second-order Hermit polynomials. But we only need to solve the augmented system once. The solving process can be further improved by using some advanced solver or acceleration techniques.

Next, we perform the accuracy comparison. The statistics for 1×1 bus case from the four algorithms are summarized in Tables IV and V for the mean value and standard deviation, respectively. The parameter settings for each case is listed in Table II. We make sure that SSCM, the first-order *statCap*, and the second-order *statCap* use the same number of random variables after the PCA operations.

TABLE VII
ERROR COMPARISON OF CAPACITANCE STANDARD DEVIATIONS AMONG SSCM, AND $statCap$ (FIRST ANDSECOND ORDER)

1×1 bus, MC(10000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	2.48%	29.34%	8.77%
Avg err	2.29%	23.38%	7.91%
2×2 bus, MC(6000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	14.28%	12.98%	25.99%
Avg err	6.11%	8.51%	6.04%
3-layer metal plane, MC(6000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	8.35%	16.26%	2.38%
Avg err	3.37%	5.06%	0.86%
3×3 bus, MC(6000) as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	23.32%	21.39%	11.75%
Avg err	3.33%	10.35%	4.38%
4×4 bus, SSCM as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	0	25.7%	6.68%
Avg err	0	16.1%	3.89%
5×5 bus, *StatCap(2nd)* as standard			
	SSCM	*statCap(1st)*	*statCap(2nd)*
Max err	–	17.5%	0
Avg err	–	7.92%	0

From these two tables, we can see that first-order *statCap*, second-order *statCap*, and SSCM give the similar results for both mean value and standard deviation compared with the MC method. For all the other cases, the times we carry out MC simulations are as shown in Table III, and the similar experimental results can be obtained. The maximum errors and average errors of mean value and standard deviation for all the testing cases are shown in Tables VI and VII. Compare to the MC method, the accuracy of the second-order *statCap* is better than the first-order *statCap* method, while from Table III, the speed of second-order *statCap* keeps in the same order as first-order *statCap*, and is still much faster than SSCM and MC.

VII. CONCLUSION

In this paper, we have proposed a novel statistical capacitance extraction method, called *statCap*, for three-3-D interconnects considering process variations. The new method is based on the orthogonal polynomial method to represent the variational geometrical parameters in a deterministic way. We consider both first-order and second-order variational effects. The new method avoids the sampling operations in the existing collocation-based spectral stochastic method. The new method solves an enlarged potential coefficient system to obtain the coefficients of orthogonal polynomials for capacitances. *statCap* only needs to set up the augmented equation once, and can exploit the sparsity and low-rank property to speedup the extraction process. The new *statCap* method can consider second-order perturbation effects to generate more accurate quadratic variational capacitances. Experimental results show that our method is two orders of magnitude faster than the recently proposed statistical capacitance extraction method based on the spectral stochastic collocation method and many orders of magnitude faster than the MC method for several practical interconnect structures.

APPENDIX

In this appendix section, we detail the derivations for computing derivatives in (40), (42), and (42).

First, we consider the scenario where panel i and panel j are far away (their distance is much larger than the panel area). In this case, the approximations in (18) and (19) are still valid. From free-space Green function, we have (21) and (22) for the first-order Hermite polynomails, and we have the following for the second-order Hermite polynomails:

$$P_{ij,0} = \frac{1}{|\vec{x}_i - \vec{x}_j|} \tag{46}$$

$$\frac{\partial P_{ij}}{\partial \Delta n_i} = -\frac{\vec{r}\cdot\vec{n_i}}{|r|^3} \tag{47}$$

$$\frac{\partial P_{ij}}{\partial \Delta n_j} = \frac{\vec{r}\cdot\vec{n_j}}{|\vec{r}|^3} \tag{48}$$

$$\frac{\partial^2 P_{ij}}{\partial {\Delta n_i}^2} = \frac{3(\vec{r}\cdot\vec{n_i})^2}{|\vec{r}|^5} - \frac{1}{|\vec{r}|^3} \tag{49}$$

$$\frac{\partial^2 P_{ij}}{\partial {\Delta n_j}^2} = \frac{3(\vec{r}\cdot\vec{n_j})^2}{|\vec{r}|^5} - \frac{1}{|\vec{r}|^3} \tag{50}$$

$$\frac{\partial^2 P_{ij}}{\partial \Delta n_j \Delta n_i} = \frac{-3(\vec{r}\cdot\vec{n_j})(\vec{r}\cdot\vec{n_i})}{|\vec{r}|^5}. \tag{51}$$

Second, we consider the scenario where panel i and panel j are near each other (their distance is comparable with the panel area). In this case, the approximation in (18) is no longer accurate, and we must consider the general form in (35) and (36).

Since panel i panel j are perpendicular to $\Delta n_i/\Delta n_j$, for $\partial P_{ij}/\partial \Delta n_j$ and $\partial^2 P_{ij}/\partial {\Delta n_j}^2$, with (35), we have

$$\begin{aligned}
\frac{\partial P_{ij}}{\partial \Delta n_j} &\approx \frac{\partial(1/s_j)\int_{S_j} G(\vec{x}_i,\vec{x}_j)da_j}{\partial \Delta n_j} \\
&= \frac{\partial(1/s_j)\int_{S_j}(1/|\vec{x}_i - \vec{x}_j + \Delta n_i - \Delta n_j|)da_j}{\partial \Delta n_j} \\
&= \frac{1}{s_j}\int_{S_j} \frac{\partial(1/|\vec{x}_i - \vec{x}_j + \Delta n_i - \Delta n_j|)}{\partial \Delta n_j} da_j \\
&= \frac{1}{s_j}\int_{S_j} \frac{\vec{r}\cdot\vec{n}_j}{|\vec{r}|^3} da_j \\
&= \frac{\vec{r}\cdot\vec{n}_j}{s_j}\int_{S_j} \frac{1}{|\vec{r}|^3} da_j \qquad (52) \\
\frac{\partial^2 P_{ij}}{\partial {\Delta n_j}^2} &\approx \frac{\partial^2(1/s_j)\int_{S_j} G(\vec{x}_i,\vec{x}_j)da_j}{\partial {\Delta n_j}^2} \\
&= \frac{\partial^2(1/s_j)\int_{S_j}(1/|\vec{x}_i - \vec{x}_j + \Delta n_i - \Delta n_j|)da_j}{\partial {\Delta n_j}^2} \\
&= \frac{1}{s_j}\int_{S_j} \frac{\partial^2(1/|\vec{x}_i - \vec{x}_j + \Delta n_i - \Delta n_j|)}{\partial {\Delta n_j}^2} da_j \\
&= \frac{1}{s_j}\int_{S_j} \frac{3(\vec{r}\cdot\vec{n}_j)^2}{|\vec{r}|^5} - \frac{1}{|\vec{r}|^3} da_j \\
&= \frac{3(\vec{r}\cdot\vec{n}_j)^2}{s_j}\int_{S_j} \frac{da_j}{|\vec{r}|^5} - \frac{1}{s_j}\int_{S_j} \frac{da_j}{|\vec{r}|^3}. \qquad (53)
\end{aligned}$$

Similarly, with (36), we can further obtain

$$\begin{aligned}
\frac{\partial P_{ij}}{\partial \Delta n_i} &\approx \frac{\partial(1/s_i)\int_{S_i} G(\vec{x}_i,\vec{x}_j)da_i}{\partial \Delta n_i} \\
&= \frac{-\vec{r}\cdot\vec{n}_i}{s_i}\int_{S_i} \frac{1}{|\vec{r}|^3} da_i \qquad (54) \\
\frac{\partial^2 P_{ij}}{\partial {\Delta n_i}^2} &\approx \frac{\partial^2(1/s_i)\int_{S_i} G(\vec{x}_i,\vec{x}_j)da_i}{\partial {\Delta n_i}^2} \\
&= \frac{3(\vec{r}\cdot\vec{n}_i)^2}{s_i}\int_{S_i} \frac{da_i}{|\vec{r}|^5} - \frac{1}{s_i}\int_{S_i} \frac{da_i}{|\vec{r}|^3}. \qquad (55)
\end{aligned}$$

While for $\partial^2 P_{ij}/\partial \Delta n_j \Delta n_i$, we need to further consider two cases. First, when panel i and panel j are in parallel, we have

$$\frac{\partial^2 P_{ij}}{\partial {\Delta n_i}^2} = \frac{\partial^2 P_{ij}}{\partial {\Delta n_j}^2} = -\frac{\partial^2 P_{ij}}{\partial \Delta n_j \Delta n_i}. \tag{56}$$

Second, we consider panel i and panel j are not in parallel. Then, we arrive

$$\begin{aligned}
\frac{\partial^2 P_{ij}}{\partial \Delta n_j \Delta n_i} &= \frac{\partial(\partial P_{ij}/\partial \Delta n_i)}{\partial \Delta n_j} \\
&= \frac{\partial(-(\vec{r}\cdot\vec{n}_i/s_i)\int_{S_i}(1/|\vec{r}|^3)da_i)}{\partial \Delta n_j} \\
&= -\frac{\vec{r}\cdot\vec{n}_i}{s_i}\frac{\partial\int_{S_i}(1/|\vec{r}|^3)da_i}{\partial \Delta n_j}. \qquad (57)
\end{aligned}$$

Assume the conductors are rectangular geometries. Then two panels should be either in parallel or perpendicular. Since panel i and panel j are not parallel, these two panels will be perpendicular.

Without loss of generality, we assume that panel i is in parallel with xz-plane and panel j is in parallel with yz-plane. Then, it is easy to see, $\vec{n}_i = (0,1,0)$ and $\vec{n}_j = (1,0,0)$. Let u_{kl}, where $k,l \in \{0,1\}$, denote the four corners of panel i, with $(x_{ik},\ y_i,\ z_{il})$ being the Cartesian cooridinates of corner u_{kl}, and the center of gravity is $(x_i,\ y_i,\ z_i)$. Let t_{kl}, $k,l \in \{0,1\}$, denote the four corners of panel j, with $(x_j,\ y_{jk},\ z_{jl})$ being the Cartesian cooridinates of corner t_{kl}, and the center of gravity is $(x_j,\ y_j,\ z_j)$.

After this, (57) can be further deduced to

$$\begin{aligned}
&\frac{\partial^2 P_{ij}}{\partial \Delta n_j \Delta n_i} \\
> \ &= \frac{y_j - y_i}{s_i}\frac{\partial\int_{x_{i0}}^{x_{i1}}\int_{z_{i0}}^{z_{i1}}(dxdz/|\vec{r}|^3)}{\partial x_j} \\
> \ &= \frac{y_j - y_i}{s_i}\frac{\partial\int_{x_{i0}-x_j}^{x_{i1}-x_j}(\int_{z_{i0}}^{z_{i1}}(dz/|\vec{r'}|^3)dx}{\partial x_j} \\
> \ &= \frac{y_j - y_i}{s_i}\left(\int_{z_{i0}}^{z_{i1}}\frac{dz}{|\vec{r-}|^3} - \int_{z_{i0}}^{z_{i1}}\frac{dz}{|\vec{r+}|^3}\right) \\
> \ &= \frac{y_j - y_i}{s_i}\sum_{k=0}^{1}\sum_{l=0}^{1}\left(\frac{(-1)^{k+l+1}(z_{il} - z_j)}{((x_{ik} - x_j)^2 + (y_i - y_j)^2)}\right. \\
> \ &\quad \left. \times\frac{1}{\sqrt{(x_{ik} - x_j)^2 + (y_i - y_j)^2 + (z_{il} - z_j)^2}}\right) \qquad (58)
\end{aligned}$$

where

$$\vec{r} = \sqrt{(x-x_j)^2+(y_i-y_j)^2+(z-z_j)^2}$$
$$\vec{r'} = \sqrt{(x)^2+(y_i-y_j)^2+(z-z_j)^2}$$
$$\vec{r^+} = \sqrt{(x_{i1}-x_j)^2+(y_i-y_j)^2+(z-z_j)^2}$$
$$\vec{r^-} = \sqrt{(x_{i0}-x_j)^2+(y_i-y_j)^2+(z-z_j)^2}$$

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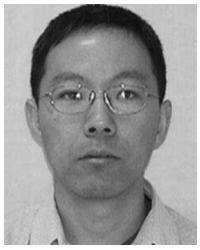

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