A Sparse Grid based Spectral Stochastic Collocation Method for Variations-Aware Capacitance Extraction of Interconnects under Nanometer Process Technology

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Abstract

In this paper, a Spectral Stochastic Collocation Method (SSCM) is proposed for the capacitance extraction of interconnects with stochastic geometric variations for nanometer process technology. The proposed SSCM has several advantages over the existing methods. Firstly, compared with the PFA (Principal Factor Analysis) modeling of geometric variations, the K-L (Karhunen-Loeve) expansion involved in SSCM can be independent of the discretization of conductors, thus significantly reduces the computation cost. Secondly, compared with the perturbation method, the stochastic spectral method based on Homogeneous Chaos expansion has optimal (exponential) convergence rate, which makes SSCM applicable to most geometric variation cases. Furthermore, Sparse Grid combined with a MST (Minimum Spanning Tree) representation is proposed to reduce the number of sampling points and the computation time for capacitance extraction at each sampling point. Numerical experiments have demonstrated that SSCM can achieve higher accuracy and faster convergence rate compared with the perturbation method.

1. Introduction

When process technology scales down to nanometer range and clock frequency goes beyond Multi-GHz, the signal integrity problem caused by non-ideal interconnects poses ever increasing challenges to today's IC design. Parasitic extraction, which extracts the parasitic parameters of these non-ideal interconnects, is now facing with the new challenges of geometric variations of interconnects. These geometric variations include CD variations, which are caused by lithography process, metal layer thickness variations and ILD (Inter-Layer Dielectric) variations, which are caused by CMP (Chemical Mechanical Polishing) process. It is predicted that such variations can reach as much as 35% at 70nm technology node [1]. A good strategy is to quantify these variations as systematic variations and random variations [2]. The systematic variations are pattern-dependent that can be modeled by some closed-form models, while the random variations, of which the sources are often unpredictable, need a more sophisticated modeling methodology to capture the random process variations effect within the parasitic extraction of interconnects.

Generally, the stochastic geometric variations can be modeled as random processes [3], resulting in a stochastic PDE problem for variation-aware capacitance extraction of interconnects. A straightforward approach for solving such a stochastic problem is Monte Carlo method, which is often regarded as a benchmark approach but suffers from hundreds of thousands of samplings. To reduce the computation cost, a non-sampling method named FastSies, which aims to capture the off-chip rough surface effect within the capacitance parameter, was proposed in [4] to solve stochastic PDE problem. This method is based on the Taylor expansion of the inverse of potential coefficient matrix, and computes the mean and variance of the capacitances.

However, mean and variance of the capacitances are only accurate and efficient for a Gaussian statistic of the resulting capacitance parameters, which corresponds to a linear model for the approximation of capacitances. Large-scale variations in nanometer process requires a high-order model to represent the nonlinear dependency of parasitic capacitances on multiple variation sources [1, 3], and limits the extensional application of FastSies to geometric variations. Therefore, another non-sampling method based on the perturbation method was proposed in [3] to generate a quadratic model for the capacitances of on-chip interconnects. This perturbation method first discretizes the surfaces of conductors by hierarchical panel refinement, and models the fluctuation of each panel as a random variable. The ensemble of these random variables is then reduced to a much smaller number of random variables by a Principle Factor Analysis (PFA) method [3]. The coefficients of the quadratic model are computed by the Taylor expansion of potential coefficient matrix. However, the PFA method in [3] depends on the number of panels of the discretized conductor surfaces and will slow down the algorithm especially when the correlation length of geometric variations is larger than the size of the conductor. Moreover, the convergence of the Taylor expansion requires the geometric variations to be small enough, which limits the perturbation method to slight variation applications.

Besides Taylor expansion, a more promising approach to approximate a stochastic function is Homogeneous Chaos expansion. The term "Homogeneous Chaos" was first defined by Wiener [5] as the span of Hermite polynomials of a Gaussian process, and then extended to a more general concept as polynomial chaos, which has been introduced to

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the circuit analysis first by J. Wang for solving a stochastic ODE problem in interconnect analysis [6] and a stochastic function approximation problem in delay modeling [7]. In this paper, we propose a more efficient Spectral Stochastic Collocation method based on Homogeneous Chaos to solve the stochastic PDE problem in the variation-aware parasitic extraction of on-chip interconnects.

Firstly, instead of PFA modeling of geometric variations, we adopt a K-L expansion [5] to generate a minimal random variable space to model the geometric variations. Compared with PFA, the discretization of K-L expansion is based on the correlation length of geometric variations, thus significantly reduces the computation cost to model the geometric variations. Secondly, Homogeneous Chaos is applied to model the capacitances of interconnects. To characterize the capacitance model parameters, a Stochastic Collocation method is proposed. Compared with the perturbation method, this spectral method consisting of Homogeneous Chaos expansion has optimal (exponential) convergence rate, and is very promising for capacitance modeling with geometric variations. Furthermore, a Sparse Grid technique, which is first proposed by Smolyak and serves as a "Blessing of dimensionality" in multi-dimensional quadrature and interpolation problems [8, 9], is used to reduce the number of collocation points compared with Monte Carlo method. To further reduce the computation cost at each collocation point, we propose a MST (Minimum Spanning Tree) representation of Sparse Grids to accelerate the convergence of GMRES at collocation points.

The rest of this paper is organized as follows. Background describing capacitance extraction problem with geometric variations and perturbation method is presented in Section 2. The main idea of the Spectral Stochastic Collocation Method (SSCM) is proposed in Section 3. Numerical results are provided in Section 4. Finally, the conclusions are drawn in Section 5.

2 Background

In this section, we first formulate the problem of capacitance extraction of interconnects with geometric variations, and then briefly review the perturbation method [3]. Finally, the Homogeneous Chaos expansion, which is the fundamental of SSCM, is presented.

2.1 Formulation of capacitance extraction

For capacitance extraction of interconnects, a variety of methods are based on a Boundary Element Method formulation [10], which involves solving the following integral equation,

$$\int_{surfaces} \frac{1}{4\pi\varepsilon_0|\vec{r}-\vec{r}\,'|}\rho(\vec{r}\,')da' = v(\vec{r}), \qquad (1)$$

where $\rho(\vec{r}\,')$ is the charge distribution on the interconnect surfaces, $v(\vec{r})$ is the potential and $\frac{1}{4\pi\varepsilon_0|\vec{r}-\vec{r}\,'|}$ is the free space Green's function. Based on the fact that the charges are restricted to the surfaces of conductors, the surfaces of conductors are first discretized into m panels, and the charge density, as well as the potential, is assumed to be constant over each panel. Hence, the contribution of the charge distributed on the j^{th} panel to the potential of the i^{th} panel is in proportion to the potential coefficient $P_{ij} = \frac{1}{4\pi\varepsilon_0 a_j}\int_{panel\ j}\frac{1}{|\vec{r}_i-\vec{r}_j|}dS_j$, where a_j is the area of the j^{th} panel and $\vec{r}_i$ is the center of the i^{th} panel [10]. Based on equation (1), the ensemble of these contributions to all panels results in a set of linear equations, which is the discrete form of the Integral Equation (IE),

$$\mathbf{P}\cdot\vec{q} = \vec{v}, \qquad (2)$$

where $\mathbf{P} \in \mathbb{R}^{m\times m}$ is the potential coefficient matrix and $\vec{q}, \vec{v} \in \mathbb{R}^{m\times 1}$ are surface charge and potential vector, respectively. The j^{th} column of the capacitance matrix is then computed by setting the voltage of j^{th} conductor to 1, grounding the other conductors and summing up the charge of panels of the corresponding conductors.

When the geometric variations are taken into account, the charges are distributed on the fluctuating surface. The variation of the i^{th} panel can be described by $\vec{r}_i + \Delta\vec{r}_i$ [3]. The term $\Delta\vec{r}_i$ denotes the fluctuation of i^{th} panel w.r.t. the nominal smooth reference surface described by $\vec{r}_i$, and is modeled as a Gaussian random process $h(\vec{r}_i)$ [2, 3]. Such a stationary Gaussian random process can be defined by two functions, i.e. the probability density function in (3) and the correlation function in (4).

$$f(h(\vec{r}_i)) = \frac{1}{\sqrt{2\pi\sigma^2}}exp(-\frac{h^2(\vec{r}_i)}{2\sigma^2}), \qquad (3)$$

$$Cov(\vec{r}_i,\vec{r}_j) = \sigma^2 exp(-\frac{|\vec{r}_i-\vec{r}_j|^2}{\eta^2}), \qquad (4)$$

where σ is the standard variance and η is the correlation length. Therefore, the resulting potential coefficient P_{ij} becomes a function of random variables $\{\Delta\vec{r}_i\}_{i=1}^m$. Note that the fluctuation of each panel is assumed to be uniform. So altogether there are m random variables for m panels. As a result, P and $\vec{q}$ in (2) are functions of these m random variables, and the IE in (2) becomes a Stochastic Integral Equation (SIE) in discrete form,

$$\mathbf{P}(\Delta\vec{r}_1,\cdots,\Delta\vec{r}_m)\cdot\vec{q}(\Delta\vec{r}_1,\cdots,\Delta\vec{r}_m) = \vec{v}. \qquad (5)$$

A traditional approach for solving SIE is using Monte Carlo method, which amounts to repeated solutions of (2) for various samplings of the random space. On the other hand, the convergence rate of Monte Carlo method is only $O(1/\sqrt{M})$, where M is the number of the samplings of the random variables. An efficient non-sampling approach proposed in [3] is a combination of hierarchical method and perturbation method as reviewed in the following.

2.2 A Perturbation method for SIE

In order to reduce the complexity of modeling geometric variations, the set of random variables $\{\Delta\vec{r}_i\}_{i=1}^m$ is first reduced to a minimal random variables space $\{\delta_i\}_{i=1}^N$ by PFA [3], where N will be much smaller than m. As a result, $\{\Delta\vec{r}_i\}_{i=1}^m$ are linear combinations of these reduced random variables $\{\delta_i\}_{i=1}^N$. A Taylor expansion of potential coefficient around $|(\vec{r}_i-\vec{r}_j)|$ results in

$$P_{ij} = \tilde{P}_{ij} + \sum_{k=1}^{N}\Delta P_{ij}^k\delta_k + \sum_{k=1}^{N}\sum_{l=1}^{N}\Delta P_{ij}^{kl}\delta_k\delta_l + \cdots, \qquad (6)$$

where $\tilde{P}_{ij}$ is the potential coefficient for smooth reference surface and the convergence of Taylor expansion requires that $\left|\frac{(\Delta\vec{r}_i-\Delta\vec{r}_j)}{(\vec{r}_i-\vec{r}_j)}\right| \ll 1$. A quadratic model for charge density is then used in [3],

$$\vec{q} = \vec{q}^{\,0} + \sum_{k=1}^{N}\Delta\vec{q}^{\,k}\delta_k + \sum_{k=1}^{N}\sum_{l=1}^{N}\Delta\vec{q}^{\,kl}\delta_k\delta_l. \qquad (7)$$

Substituting (6) and (7) into (5) and matching the coefficients up to the second order yield the recursion of the coefficients $\vec{q}^{\,0}$, $\Delta\vec{q}^{\,k}$ and $\Delta\vec{q}^{\,kl}$ [3]. Then the capacitance can be computed accordingly.

There are two limitations of this approach. One is related to the PFA method [3], which is in fact an eigen-decomposition problem of the correlation matrix associated with the discretization of the conductor surfaces. The eigenvalue problem of such a correlation matrix can result in an $O(m^3)$ complexity, where m is the number of panels, and becomes the bottleneck of the algorithm. The other limitation is the convergence condition of Taylor expansion, $\left|\frac{(\Delta\vec{r}_i-\Delta\vec{r}_j)}{(\vec{r}_i-\vec{r}_j)}\right| \ll 1$, which limits the application of the perturbation method to slight geometric variations.

2.3 Homogeneous Chaos Expansion

An alternative approach to approximate a stochastic function is Homogeneous Chaos expansion.

***Theorem** 1 The Homogeneous Chaos expansion (8) converges to any random process with finite second-order moments.*

$$F(\vec{\xi}) = \sum_{i_1+\cdots+i_d=0}^{\infty} f_{i_1,\cdots,i_d} H_d^{i_1,\cdots,i_d}(\vec{\xi}). \tag{8}$$

where $H_d^{i_1,\cdots,i_d}(\vec{\xi}) = H_1^{i_1}(\xi_1)\times\cdots\times H_1^{i_d}(\xi_d)$ denotes the d-dimensional Hermite polynomial of order $(i_1+\cdots+i_d)$, H_1^j is the one-dimensional Hermite polynomial of order j and

$$f_{i_1,\cdots,i_d} = \int F(\vec{\xi}) H_d^{i_1,\cdots,i_d}(\vec{\xi})\rho(\vec{\xi})d\vec{\xi}. \tag{9}$$

Term $\rho(\vec{\xi})$ corresponds to the probability density function of Gaussian random vector $\vec{\xi}$. Since most of the physical process is second-order process, the Homogeneous Chaos expansion is a better way to represent stochastic functions.

The new development of Homogeneous Chaos is the Askey scheme [11], which consists of different kinds of orthogonal polynomials with weighting functions related to different kinds of stochastic processes. Based on the Askey principle, expansion based on Hermite polynomials has the optimal (exponential) convergence rate for a Gaussian random process. When modeling other non-Gaussian random fields, the corresponding Askey scheme polynomial chaos can be chosen in order to achieve the optimal convergence rate. Take a Poisson process for example, either Homogeneous Chaos expansion or Taylor expansion will have a lower convergence rate than Charlier-chaos expansion. In this paper, we first deal with the most common Gaussian variations and propose to employ Homogeneous Chaos to model the capacitances with geometric variations.

3 Spectral Stochastic Collocation Method

In this section, we will propose a Spectral Stochastic Collocation Method (SSCM), as one of the stochastic spectral methods, for variation-aware capacitance extraction of interconnects. First, instead of a PFA procedure, a K-L expansion procedure is adopted to find a minimal random variable space to model the geometric variations, as will be presented in subsection 3.1. Then spectral stochastic collocation method is proposed in subsection 3.2. Finally, the Sparse Grid technique with Minimum Spanning Tree (MST) representation, which significantly reduces the sampling points and the computation time, is developed for stochastic collocation method in subsection 3.3.

3.1 K-L Expansion

The PFA [3] and K-L expansion [5] are both used to find a small number of random variables to model geometric variations, and therefore reduce the complexity. K-L expansion is the one that directly applies to a random process,

$$h(\vec{r}) \approx \sum_{n=1}^{N} \sqrt{\lambda_n}\xi_n g_n(\vec{r}), \tag{10}$$

where $\{\xi_n\}_{n=1}^N$ is a set of independent random variables with $N(0,1)$ distribution when the surface fluctuation $h(\vec{r})$ is a Gaussian random process, λ_n is the n^{th} largest eigenvalue of the correlation function $Cov(\vec{r}_1,\vec{r}_2)$ defined in (4) and $g_n(\vec{r})$ is the corresponding eigenfunction, i.e.

$$\int_\Omega Cov(\vec{r}_1,\vec{r}_2)g_n(\vec{r}_2)d\vec{r}_2 = \lambda_n g_n(\vec{r}_1), \tag{11}$$

where Ω denotes the area of conductor surface. The N-term approximation in (10) possesses the following best approximation property.

***Theorem** 2 (10) is the best root mean square approximation of the random process $h(\vec{r})$ [5].*

Equation (11) is a homogeneous Fredholm Equation of the second kind, and many numerical techniques have been proposed to solve such an equation. In this paper, the popular Nystrom method [12] is used.

The advantage of K-L expansion over PFA is that spectral decomposition is directly applied to the correlation function instead of the correlation matrix. Therefore, we are able to adopt a different discretization scheme based on the correlation length to solve (11) in order to keep the balance between accuracy and efficiency. Since the correlation length is much longer than the size of conductors for most on-chip geometric variations, the amount of unknowns, i.e. p, required for the discretization of (11) can be much smaller than m, where m is the amount of panels for the discretization of conductor surfaces. Furthermore, an eigenvalue problem has a cubic complexity, thus m/p times saving in the amount of panels can result in $(m/p)^3$ times saving in computation time.

Now, we have the geometric variations modeled by a small number of random variables $\vec{\xi}$. The normal-direction fluctuation of the i^{th} panel, $\Delta\vec{r}_i = h(\vec{r}_i)$, is approximated by a linear function of these random variables (10). Therefore, P and $\vec{q}$ in (5) become functions of these reduced set of random variables, and SIE in (5) can be re-written as

$$\mathbf{P}(\xi_1,\cdots,\xi_N)\vec{q}(\xi_1,\cdots,\xi_N) = \vec{v}. \tag{12}$$

3.2 Stochastic Collocation Method

For solving a stochastic equation like (12), spectral methods based on polynomial chaos, including Galerkin and collocation method, possess exponential convergence rate [11]. In this paper, the more efficient collocation method, which simply consists of the following two steps, is applied to the capacitance extraction with geometric variations.

1) Homogeneous Chaos is employed for the discretization of unknowns $\vec{q}(\vec{\xi})$ in random space,

$$\vec{q}(\vec{\xi}) \approx \tilde{q}(\vec{\xi}) = \sum_{i_1+\cdots+i_d\le 2} \vec{q}_{i_1,\cdots,i_d} H_d^{i_1,\cdots,i_d}(\vec{\xi}), \tag{13}$$

where $H_d^{i_1,\cdots,i_d}(\vec{\xi})$ denotes the Hermite polynomials of order at most two for a quadratic modeling and $\vec{q}_{i_1,\cdots,i_d}$ are the unknown coefficients.

2) To compute the unknown coefficients in (13), the inner product of test delta function and the residue, $R(\vec{\xi}) =$

$\mathbf{P}(\vec{\xi})\tilde{q}(\vec{\xi}) - \vec{v}$, is enforced to vanish at each collocation point $\hat{\xi}^i$, i.e.

$$< \mathbf{P}(\vec{\xi})\tilde{q}(\vec{\xi}) - \vec{v}, \delta(\vec{\xi} - \hat{\xi}^i) >_\rho = \mathbf{P}(\hat{\xi}^i)\tilde{q}(\hat{\xi}^i) - \vec{v} = 0, \quad (14)$$

where $i = 1, \cdots, M$ and $< >_\rho$ is the inner product for random space. For one-dimensional problems, Gaussian points are generally used for collocation points, when extended to high-dimensional cases, we choose Sparse Grids as collocation points, which will be explained in Section 3.3.

Equations (15) and (16) can be derived by setting (13) and (14) at M collocation points.

$$\sum_{i_1+\cdots+i_d \le 2} \vec{q}_{i_1,\cdots,i_d} H_d^{i_1,\cdots,i_d}(\hat{\xi}^i) = \tilde{q}(\hat{\xi}^i), \quad (15)$$

$$\tilde{q}(\hat{\xi}^i) = \mathbf{P}(\hat{\xi}^i)^{-1}\vec{v}, i = 1, \cdots, M. \quad (16)$$

Note that equations in (16) at M collocation points are naturally decoupled. Therefore, we first compute the charges at collocation points by solving (16), and then evaluate the unknown coefficients $\vec{q}_{i_1,\cdots,i_d}$ from (15).

Equation (16) becomes a conventional IE at each collocation point, and will be solved by an iterative method such as GMRES, combined with fast solvers using preconditioning and Hierarchical method [13, 14], resulting in $O(m)$ complexity, where m is the number of panels.

In order to compute the unknown coefficients from (15), we first derive the solution of the k^{th} equation in (15), i.e.

$$\sum_{i_1+\cdots+i_d \le 2} q^k_{i_1,\cdots,i_d} H_d^{i_1,\cdots,i_d}(\hat{\xi}^i) = q^k(\hat{\xi}^i), \; i{=}1,\cdots,M, \quad (17)$$

where $q^k_{i_1,\cdots,i_d}$ and $q^k(\hat{\xi}^i)$ denote the k^{th} element of vector $\vec{q}_{i_1,\cdots,i_d}$ and $\tilde{q}(\hat{\xi}^i)$, respectively. (17) can be rewritten as

$$\mathbf{A}\vec{x}_k = \vec{b}_k, \quad (18)$$

$$where\ \mathbf{A} = \begin{bmatrix} H_d^{0,\cdots,0}(\hat{\xi}^1) & H_d^{1,\cdots,0}(\hat{\xi}^1) & \cdots & H_d^{0,\cdots,2}(\hat{\xi}^1) \\ \vdots & \vdots & \ddots & \vdots \\ H_d^{0,\cdots,0}(\hat{\xi}^M) & H_d^{1,\cdots,0}(\hat{\xi}^M) & \cdots & H_d^{0,\cdots,2}(\hat{\xi}^M) \end{bmatrix},$$

$$\vec{x}_k = \left[q^k_{0,\cdots,0} q^k_{1,\cdots,0} \cdots q^k_{0,\cdots,2}\right]^T, \vec{b}_k = \left[q^k(\hat{\xi}^1) \cdots q^k(\hat{\xi}^M)\right]^T.$$

For a multi-dimensional problem, the number of collocation points M is generally larger than the number of unknown coefficients. Therefore, a weighted Least Square method is applied to (18) for the computation of unknown coefficients $q^k_{i_1,\cdots,i_d}$, and the solution is

$$\vec{x}_k = \left(\mathbf{A}^T\mathbf{W}\mathbf{A}\right)^{-1}\mathbf{A}^T\mathbf{W}\vec{b}_k, \quad (19)$$

where $\mathbf{W} = diag(w_1, \cdots, w_M)$ are the corresponding weights of Sparse Grids, as will be explained in section 3.3. Based on the orthonormality of Hermite polynomials, $\mathbf{A}^T\mathbf{W}\mathbf{A} = \mathbf{I}$. Therefore, by employing (19) as the solution of (17) for $k = 1, \cdots, m$, the solution of (15) is simple as

$$\vec{q}_{i_1,\cdots,i_d} = \sum_{i=1}^{M} \tilde{q}(\hat{\xi}^i) H_d^{i_1,\cdots,i_d}(\hat{\xi}^i) w_i, \;\; i_1+\cdots+i_d \le 2. \quad (20)$$

The resulting unknown coefficients $\{\vec{q}_{i_1,\cdots,i_d}\}_{i_1+\cdots+i_d\le 2}$ in (20) are exactly the coefficients of a Homogeneous Chaos expansion of $\tilde{q}(\vec{\xi})$, as defined in (8) and (9), while the integration for coefficients in (9) is now computed by a Sparse Grid quadrature in (20), as will be explained in the following.

3.3 Sparse Grid Technique

For multi-dimensional integration, Sparse Grid develops a minimal number of collocation points based on one-dimensional Gaussian quadrature and avoids the exponential growth of computation cost w.r.t. the dimensionality [8, 9, 15]. Furthermore, a MST (Minimum Spanning Tree) representation for Sparse Grids is developed, further reducing the computation cost at each collocation point.

3.3.1 One-dimensional Gaussian Quadrature

Gaussian-Hermite quadrature can be represented by the following equation [12],

$$\frac{1}{\sqrt{2\pi}} \int_\Gamma e^{-\frac{x^2}{2}} f(x)dx = \sum_{i=1}^{l+1} f(x_i^{l+1}) w_i^{l+1}, \quad (21)$$

where Γ is the integration domain, $f(x)$ is the integrand, x_i^{l+1} and w_i^{l+1} are the collocation point and weight, respectively. It can be proved that the quadrature (21) is exact for all polynomials of degree at most $(2l+1)$ if the quadrature points are selected as the roots of $(l+1)^{th}$-order Hermite polynomial [12]. In this paper, a l-level accuracy Gaussian quadrature rule refers to the quadrature formula constructed by the roots of $(l+1)^{th}$-order orthogonal polynomial.

3.3.2 Sparse Grid for Multi-dimensional Quadrature

Let $\Theta_1^l = \{x_1^l, \cdots, x_l^l\}$ and $W_1^l = \{w_1^l, \cdots, w_l^l\}$ denote the set of collocation points and weights for one-dimensional $(l-1)$-level accuracy Gaussian quadrature rule. Direct tensor product of Θ_1^l and W_1^l can extend the quadrature formula (21) to multi-dimensional integration, but suffers from the "Curse of Dimensionality" [9]. The amount of collocation points is $(k+1)^d$ when applied to a d-dimensional integration of k-level accuracy, which makes the direct tensor product impracticable.

A more promising approach for multi-dimensional integration is the Sparse Grid [15], of which the quadrature points Θ_d^k for a d-dimensional quadrature of k-level accuracy is constructed by a linear combination of the tensor product of Θ_1^l,

$$\Theta_d^k = \bigcup_{k+1 \le i_1+\cdots+i_d \le d+k} (\Theta_1^{i_1} \times \cdots \times \Theta_1^{i_d}), \quad (22)$$

with the corresponding weight,

$$w^{i_1,\cdots,i_d}_{j_{i_1},\cdots,j_{i_d}} = (-1)^{d+k-|\vec{i}|}\binom{d-1}{d+k-|\vec{i}|}(w^{i_1}_{j_{i_1}} \cdots w^{i_d}_{j_{i_d}}). \quad (23)$$

Then, integration is computed as a summation of the contributions at Sparse Grids,

$$\left(\tfrac{1}{\sqrt{2\pi}}\right)^d \int e^{-\frac{x_1^2+\cdots+x_d^2}{2}} f(x_1, \cdots, x_d)dx_1 \cdots dx_d$$
$$= \sum_{(\hat{x}^{i_1}_{j_{i_1}}, \cdots, \hat{x}^{i_d}_{j_{i_d}}) \in \Theta_d^k} f(\hat{x}^{i_1}_{j_{i_1}}, \cdots, \hat{x}^{i_d}_{j_{i_d}}) w^{i_1,\cdots,i_d}_{j_{i_1},\cdots,j_{i_d}}. \quad (24)$$

***Theorem** 3 Sparse Grid quadrature is exact for all d-variables polynomials of order at most $(2k+1)$ [15].*

Therefore, in this paper, Θ_d^2 is applied to the quadratic modeling of capacitance while Θ_d^1 is used for the linear modeling.

Furthermore, the amount of Sparse Grids for d-dimensional quadrature of k-level accuracy is [15],

$$M = dim(\Theta_d^k) \sim \frac{2^k}{k!}d^k \sim 2^k dim(\pi_d^k), \; d \gg 1, \quad (25)$$

where π_d^k denotes the space of all d-variables Hermite polynomials of order at most k. The algorithm may be regarded as optimal because at least $dim(\pi_d^k)$ collocation points are necessary to determine a polynomial in π_d^k. Table 1 shows the number of collocation points of different methods, an exponentially increasing rate of direct tensor product method can be observed while the number of second-order Sparse Grids is only about four times of $dim(\pi_d^2)$.

Table 1. Amount of collocation points

(Z_d^k denotes the collocation points of direct tensor product)

d	$dim(\pi_d^1)$	Θ_d^1/Z_d^1	$dim(\pi_d^2)$	Θ_d^2/Z_d^2
6	7	13/64	28	85/729
14	15	29/16384	120	421/4782969

3.3.3 MST Structure representation of Sparse Grids

In collocation method, equation (16) has to be solved at M collocation points. In order to accelerate the convergence of GMRES for (16), charges computed at the previous nearest collocation points will be selected and serve as the initial value of GMRES at the latter collocation points. Based on this idea, we proposed to build a tree T to represent the Sparse Grids, by which capacitances at the root of T will be computed first and the capacitances at node-i in T will be computed by setting the solution of its parent node-$p(i)$ as the initial value in GMRES. In the following, we will first define the experimental distance function $d(i,j)$, which is a measurement of the computation cost of GMRES at node-i when setting the solution of node-j as its initial value, and then derive a Minimum Spanning Tree to minimize the total cost of GMRES at collocation points.

Experimental distance function:

It is observed that charges at surfaces of two different collocation points are close in value when the shapes of surfaces are close to each other. Moreover, it will be efficient for GMRES when using an initial value close to the real solution. Therefore, the similarity of surface shapes at node-i and node-j can be reasonably used to quantify the computation cost of GMRES at node-i when setting the solution of node-j as its initial value.

Let $\hat{\xi}^i = (\xi_1^i, \cdots, \xi_N^i)$ and $\hat{\xi}^j = (\xi_1^j, \cdots, \xi_N^j)$ be two collocation points of the Sparse Grids. Based on K-L expansion (10), the difference of $h(\vec{r})$ at $\vec{r}$ between two collocation points is $\Delta_{ij}h(\vec{r}) = \sum_{n=1}^{N}\sqrt{\lambda_n}(\xi_n^i - \xi_n^j)g_n(\vec{r})$. Therefore, the experimental distance function can be defined by

$$d(i,j) = \int_\Omega [\Delta_{ij}h(\vec{r})]^2 d\vec{r} = \sum_{n=1}^{N}\lambda_n(\xi_n^i - \xi_n^j)^2, \qquad (26)$$

where Ω is the area of conductor surfaces.

MST representation of Sparse Grids:

Borrowing the idea from the graph theory [16], Sparse Grids can be represented by a complete undirected graph $G = (V, E)$, where the vertex set V contains all the collocation points. For edge between node-i and node-j, an experimental distance function $d(i,j)$ is defined in (26) to quantify the computation cost of GMRES at node-i when setting the solution of node-j as the initial value for node-i.

Therefore, the total cost of GMRES at collocation points of a tree T generated from graph G can be estimated by $\sum_{i=1}^{M} d(i,p(i))$, where node-$p(i)$ is the parent node of node-i and M is the number of collocation points. A Minimum Spanning Tree (MST), of which $\sum_{i=1}^{M} d(i,p(i))$ is minimal, can minimize the total computation cost of GMRES at collocation points.

Kruskal's algorithm and Prim's algorithm can be applied to grow a MST from the graph G [16]. Capacitance extraction for each collocation points can then be carried out by a Depth-First Search of the MST. The charge density of the parent node is set as the initial value of GMRES for the capacitance extraction of the child node.

4 Numerical Results

In this section, two 3-D test cases, which are 3-bit bus and 2x2 bus, are used to validate the accuracy and efficiency of the proposed SSCM. Considering the 35% variations at 70nm technology node [1], the 3σ range of geometric variations of interconnects, including width variations and thickness variations, is chosen as 30% of the dimension of conductors in 3-bit bus example and 35% in 2x2 bus example. In these cases, the correlation length of width variations is assumed to be 27 times of the conductor width, while the correlation length of thickness variations is set as 40 times of the conductor width. Either PFA or K-L expansion preserves two and four random variables to model the width variations and thickness variations, respectively. Monte Carlo method with 50,000 samplings are used as a benchmark of the experiments.

A) Efficiency of K-L Expansion

In Table 2, computation costs for PFA and K-L expansion for various on-chip interconnect structures are compared. Since the discretization of K-L expansion is based on the correlation length of geometric variations, the number of unknowns p in K-L expansion can be much smaller than the number of panels m in PFA, as shown in Table 2. Up to two orders of computation time saving by K-L expansion can be observed.

Table 2. Computation time of K-L and PFA

test cases	PFA		KL	
	m	cost time	p	cost time
3-bit bus	1440	9.71	272	0.05
2x2 bus	528	1.08	48	0.005

B) Accuracy and Efficiency of SSCM

Figure 1 is a comparison of the Cumulative Distribution Functions (cdf) of the self-capacitance of the mid-conductor C_{22} in 3-bit bus example. Compared with the perturbation result, the overall SSCM result is more close to the Monte Carlo simulation.

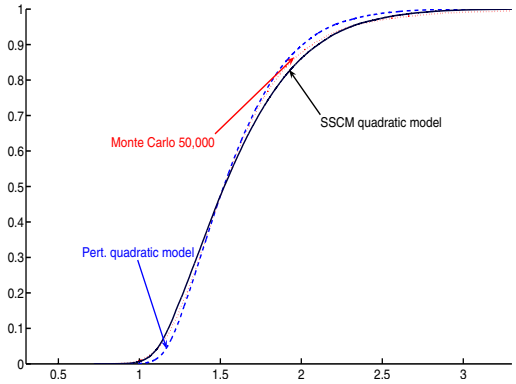

Figure 1. CDF of C_{22} in 3-bit bus example

For further comparison, the mean values, variances and covariances of the capacitances of both test cases are listed in Table 3-5. It is observed that,

1) The quadratic model of SSCM has a great improvement in the accuracy compared with the linear model, while the

accuracy improvement of perturbation method from linear model to quadratic model is not so significant.
2) For the approximation of means, variances and covariances, linear model of SSCM has the same order of accuracy compared with the quadratic model of perturbation method.

The above two points have fully demonstrated that SSCM has the optimal (exponential) convergence rate compared with perturbation method. The errors of covariances reach as much as 30% for quadratic model of perturbation method, which is far from accurate for the real application. On the other hand, quadratic model of SSCM has only within 6% errors for the approximation of covariances.

Iterations in GMRES for various methods are also listed in Table 6, which shows that,
1) Both perturbation method and SSCM have $1000\times$ *speedup compared with the Monte Carlo sampling.*
2) Compared with the SSCM without MST, SSCM based on MST representation can achieve the same accuracy while costs only half of the computation time for quadratic models in both cases.
3) With the same model order, SSCM based on MST representation has the same order of computation cost compared with the perturbation method.

In conclusion, with almost the same computation time, quadratic model of SSCM with MST has much higher accuracy than the quadratic model of perturbation method. To approximate the means, variances and covariances of the stochastic capacitance parameters, linear model of SSCM with/without MST representation can achieve the same accuracy but with nearly one order less computation time than second-order perturbation method. Thus, the above numerical results have well demonstrated that SSCM has higher accuracy and faster convergence rate than perturbation method.

Table 3. Mean $\bar{C} = E(C)$

		MC	error of Pert.		error of SSCM	
			linear	quad.	linear	quad.
3-bit bus	C_{11}	1.14	3.46%	0.87%	0.51%	0.09%
	C_{22}	1.60	4.88%	1.11%	0.71%	0.14%
	C_{12}	-0.7	5.61%	1.28%	0.82%	0.16%
2x2 bus	C_{11}	1.17	3.58%	1.16%	0.40%	0.03%
	C_{12}	-0.7	5.73%	1.68%	0.65%	0.04%

Table 4. Variance $\sigma = \sqrt{E(C-\bar{C})^2}$

		MC	error of Pert.		error of SSCM	
			linear	quad.	linear	quad.
3-bit bus	C_{11}	0.21	19.9%	18.0%	16.0%	4.1%
	C_{22}	0.39	21.8%	19.4%	17.8%	4.6%
	C_{12}	0.20	21.9%	19.5%	18.0%	4.8%
2x2 bus	C_{11}	0.23	19.5%	17.8%	14.5%	3.4%
	C_{12}	0.21	21.8%	19.6%	16.8%	4.0%

Table 5. Covariance $\sigma^2_{i,j}=E(C_i-\bar{C}_i)(C_j-\bar{C}_j)$

		MC	error of Pert.		error of SSCM	
			linear	quad.	linear	quad.
3-bit bus	$\sigma^2_{11,22}$	0.08	34.9%	31.9%	28.2%	5.8%
	$\sigma^2_{12,22}$	-0.07	36.4%	33.1%	29.7%	6.2%
	$\sigma^2_{11,12}$	-0.04	35.1%	32.1%	28.6%	6.1%
2x2 bus	$\sigma^2_{11,22}$	0.05	32.8%	30.5%	24.3%	4.0%
	$\sigma^2_{11,12}$	-0.05	34.6%	31.9%	26.1%	4.4%

5 Conclusions

In this paper, a Spectral Stochastic Collocation Method is proposed to build a variational model of capacitance based on the Homogeneous Chaos expansion. Firstly, the K-L expansion involved in SSCM is independent of the discretization of the surfaces of conductors, thus is much more efficient than the PFA method [3]. Secondly, compared with the perturbation method based on a Taylor expansion, stochastic spectral methods consisting of Homogeneous Chaos expansion has exponential convergence rate. Furthermore, Sparse Grid combined with MST representation significantly reduces the number of collocation points and the number of iterations, and makes the SSCM very efficient. The proposed method can be further extended to non-Gaussian geometric variation cases. For random process listed in Askey scheme, the corresponding Askey polynomial chaos can be applied. While for those not listed in Askey scheme, we can also transform them to a Gaussian random process. In the future work, we will further study the SSCM for non-Gaussian variations.

Table 6. Total iterations in GMRES

	3-bit bus		2x2 bus	
	linear	quad.	linear	quad.
MC sampling	2,867,559		3,482,716	
Pert. method	452	3,182	558	3714
SSCM without MST	654	4,738	884	6284
SSCM with MST	468	2,744	588	3652

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