Solution of Dual Stochastic Static Formulations Using Double Orthogonal Polynomials

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The solution of stochastic partial differential equations (PDEs) using the spectral stochastic finite-element method (SSFEM) can lead to a very large linear system of equations. If the random input data are independent, it can be shown that the initial linear system can be split into smaller independent linear systems by using double orthogonal polynomials. In this paper, we propose the use of this approach in the case of dual potential formulations in electrokinetics. The method is applied to an electrokinetic problem taking into account the uncertainties on contact resistances.

***Index Terms*—Electromagnetism, orthogonal polynomials, random variables, spectral stochastic finite-element method (SSFEM).**

I. Introduction

THE spectral stochastic finite-element method (SSFEM) can be used to solve the stochastic static electromagnetics problem. This method has originally been proposed in mechanics by Ghanem [1] in the early 1990s and has recently been applied to solution of stochastic static electromagnetics problems [2], [3]. The method is very accurate but requires the solution of a large linear system. The number of unknowns in the system is equal to the product of the number of degrees of freedom (DoFs), N required to discretize the spatial dimension (spatial mesh), and the number of DoFs $P_{\rm out}$ required to discretize the random dimension. Even though the system to solve has special properties, its solution can be tricky when the number of random input variables is greater than about a dozen. If the randomness is in the behavior laws and the input random variables are independent, it has been shown by Babuska *et al.* [4] that using special polynomials (so-called double orthogonal polynomials) as the basis of discretization of the random dimension, the SSFEM yields $P_{\rm out}$ independent equation systems of size N. The double orthogonal polynomials have been previously used to solve the scalar potential formulation in static electromagnetics [5]. Here, we propose to solve the dual potential formulations using double orthogonal polynomials. Some properties related to power bound are pointed out in the process.

In the first part, the dual potential formulations are presented in the stochastic case. In the second part, the method of construction of the multivariate double orthogonal polynomials is detailed. In the third part, we show how to define the deterministic problem to solve starting with the expression of the double orthogonal polynomials. Finally, an example is treated.

II. Description of the Stochastic Problem

On a contractible domain D with a boundary S, the electrokinetic problem can be written as

$$\mathrm{div}\,\mathbf{J} = 0 \tag{1}$$

$$\mathbf{curl}\ \mathbf{E} = 0. \tag{2}$$

Boundary conditions are imposed on S. To simplify the problem, we will assume that we have only two disjoint surfaces S_{E1} and S_{E2} ($S_E = S_{E1} \cup S_{E2}$) on which

$$\mathbf{Exn} = \mathbf{0} \tag{3}$$

with $\mathbf{n}$ the outward unit vector on S. On the complement of S_E, denoted S_J, we have

$$\mathbf{J} \cdot \mathbf{n} = 0. \tag{4}$$

The behavior law can be written on D as

$$\mathbf{E} = \rho(x,\theta)\mathbf{J}. \tag{5}$$

$\rho(x,\theta)$ is the random resistivity with the outcome θ belonging to the space Ω. We will assume that the resistivity is equal to a random variable $\rho_q(\theta)$ on M disjoint subdomains D_q of D

$$\rho(x,\theta) = \sum_{q=1}^{M} \rho_q(\theta) I_q(x) \tag{6}$$

where $I_q(x)$ is a function that is equal to 1 on the subdomain D_q and 0 elsewhere. Since the resistivity is random, $\mathbf{E}$ and $\mathbf{J}$ are random fields. To solve the previous problems, two potential formulations can be used. Since, $\mathbf{E}$ (x,θ) is curl free, it can be written as the gradient of a scalar function $\varphi(x,\theta)$. The equation to solve is then

$$div[\rho^{-1}(x,\theta)\mathbf{grad}\varphi(x,\theta)] = 0. \tag{7}$$

We have Neumann boundary conditions on S_J and Dirichlet type on S_E with

$$\varphi(x,\theta) = 0 \text{ on } S_{E1} \quad \varphi(x,\theta) = V \text{ on } S_{E2}. \tag{8}$$

To obtain an unknown with homogeneous boundary conditions, we consider a field $\boldsymbol{\beta}(x)$ on D such that $\boldsymbol{\beta}(x)$ satisfies (2) and (3) and such that the circulation of $\boldsymbol{\beta}(x)$ from S_{E1} to S_{E2} is equal to 1. We now consider the new problem with the scalar potential $\varphi'(x,\theta)$ and with homogenous boundary conditions on S_E

$$div[\rho^{-1}(x,\theta)\mathbf{grad}\varphi'(x,\theta)] = -V div[\rho^{-1}(x,\theta)\beta(x)]. \tag{9}$$

If we denote $I(\theta)$ the current flowing through S_{E1} and S_{E2}, this current can be calculated as

$$I(\theta) = -\int_D \mathbf{J}(x,\theta) \cdot \boldsymbol{\beta}(x) dD. \tag{10}$$

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Since $\mathbf{J}(x,\theta)$ is divergence free, $\mathbf{J}(x,\theta)$ can be written as the curl of the vector potential $\mathbf{T}(x,\theta)$. The equation to solve is then

$$\mathbf{curl}[\rho(x,\theta)\mathbf{curl}\ \mathbf{T}(x,\theta)] = \tilde{0} \tag{11}$$

$\mathbf{T}(x,\theta)$ has nonhomogenous boundary conditions on S_J. We therefore introduce a field $\mathbf{N}(x)$ satisfying (1) and (4) such that the flux of $\mathbf{N}(x)$ through the surface S_{E2} is equal to 1. It can be shown that the problem to solve is

$$\mathbf{curl}[\rho(x,\theta)\mathbf{curl}\ \mathbf{T}'(x,\theta)] = -I\ \mathbf{curl}[\rho(x,\theta)\mathbf{N}(x)] \tag{12}$$

where $\mathbf{T}'$ is the unknown with homogeneous boundary conditions. The voltage $V(\theta)$ can be calculated using the following equation:

$$V(\theta) = -\int_D \mathbf{E}(x,\theta)\cdot\mathbf{N}(x)dD. \tag{13}$$

If the voltage is known, then (13) provides an additional equation required to calculate the value of the current. If the voltage has a deterministic value V, the current is then a random variable $I(\theta)$.

III. Approximation of the Potentials Using Double Orthogonal Polynomials

In the following, we detail the solution of the vector potential formulation. In the deterministic case, the vector potential $\mathbf{T}'$ is approximated using edge shape functions. Let us denote N_1 the set of edges, N_1^0 the sets of edges not located on S_J, and $\mathbf{w}_a\ (x)$ the function associated with the edge a. The cardinal of the set N_1^0 will also be denoted N_1^0. We will denote $W_1^0\ (D)$ the space generated by the functions associated with the edges belonging to N_1^0. Functions in $W_1^0\ (D)$ have naturally homogeneous boundary conditions (3) on S_J.

We consider the space of functions X depending on the random variables $\rho_1\ (\theta),\ldots,\rho_M\ (\theta)$ such that the variance exists. To approximate this space, we will consider a set of P_{out} multivariate orthogonal polynomials $(H_i\ (x_1,\ldots x_M))_{1\le i\le P_{\text{out}}}$

$$E[H_i(\rho_1[\theta]\ldots,\rho_M[\theta])H_j(\rho_1[\theta]\ldots,\rho_M[\theta])] = 0, \quad \text{if } i\neq j \tag{14}$$

with $E[\,]$ the expectation. We will denote $W_{P\text{out}}\ (\Omega)$ the space generated by this set of polynomials. Various methods have been proposed to define these polynomials. The most common polynomials used are the multivariate polynomial based on the Askey scheme [6]. We are looking for an approximation of the vector potential $\mathbf{T}'$ in the space $W_0^0(D)\otimes W_{P_{\text{out}}}\ (\Omega)$, so that $\mathbf{T}'$ can be written as $(H_i\ (\rho_1[\theta]\ldots,\rho_M[\theta])$ will be denoted $H_i(\theta)$ in the following:

$$\mathbf{T}'(x,\theta) = \sum_{a=1}^{N_1^0}\sum_{j=1}^{P_{\text{out}}} T'_{aj}\mathbf{w}_a(x)H_j(\theta) \tag{15}$$

where T'_{ij} are the degrees of freedom we need to determine. Applying the Galerkin method to a weak form of (11) leads to $N_n^0\times P_{\text{out}}$ linear equations

$$\mathbf{S}\ \mathbf{T}' = \mathbf{F} \tag{16}$$

where $\mathbf{S}$ is an $(\mathbf{N}_1^0\times P_{\text{out}})\times(N_1^0\times P_{\text{out}})$ square matrix and $\mathbf{F}$ an $(\mathbf{N}_1^0\times P_{\text{out}})$ vector. The vector $\mathbf{T}'$ is the vector of the DoFs T'_{ij}. Using (6) for the resistivity allows us to rewrite the equation system in a different way [3]. We denote the matrices $\mathbf{S}_q$ and $\mathbf{D}_q$, the vectors $\mathbf{F}_q$ and the Σ_q with the coefficients

$$\begin{aligned}
s_{ni}^q &= (I_q(x)\mathbf{curl}\mathbf{w}_i(x),\mathbf{curl}\mathbf{w}_n(x))_D\\
&\quad q\in[1,M],\qquad (i,n)\in[1,N_1^0]^2\\
d_{mj}^q &= E[\rho_q(\theta)H_j(\theta)H_m(\theta)]\\
&\quad q\in[1,M],\qquad (j,m)\in[1,P_{\text{out}}]^2\\
f_n^q &= V(I_q(x)\mathbf{N}(x),\mathbf{curl}\mathbf{w}_n(x))_D\\
&\quad q\in[1,M],\qquad n\in[1,N_1^0]\\
\Sigma_m^q &= E[\rho_q(\theta)H_m(\theta)]\\
&\quad q\in[1,M],\qquad m\in[1,P_{\text{out}}].
\end{aligned}$$

Then, using the Kronecker product $\otimes$, (16) can be written in the form [3]

$$\mathbf{S} = \sum_{q=1}^{M}\mathbf{D}_q\otimes\mathbf{S}_q \quad \mathbf{F} = \sum_{q=1}^{M}\Sigma_q\otimes\mathbf{F}_q. \tag{17}$$

The size of the linear system (17) can become very large even with a coarse mesh. If the random variables $\rho_q\ (\theta)$ are independent, we can take advantage of this property by using double orthogonal polynomials $H_i\ (\theta)$ which enables us to get a diagonal matrix $\mathbf{D}_q$. In that case, we have to solve P_{out} linear systems of size $N_1^0\times N_1^0$ instead of the whole system (16).

To construct the multivariate double orthogonal polynomials, we will first construct for each random variable $\rho_q\ (\theta)$ a set of polynomials $[h_q^j]_{1\le j\le p_{\text{out}}+1}$ such that

$$h_q^j(x) = \sum_{i=1}^{p_{\text{out}}+1} h_q^{ji}x^i \tag{18}$$

and which fulfill the following conditions:

$$E[h_q^n(\rho_q[\theta])h_q^m(\rho_q[\theta])] = \delta_{nm} \tag{19a}$$

$$E[\rho_q[\theta]h_q^n(\rho_q[\theta])h_q^m(\rho_q[\theta])] = 0, \qquad \text{if } m\neq n. \tag{19b}$$

The first relation is a feature of orthogonal polynomials but the second is an additional relation. To calculate the coefficients, we construct a matrix $\mathbf{H_q}$ $(p_{\text{out}}+1)\times(p_{\text{out}}+1)$ storing h_q^{ij}. According to (19a) and (19b) it can be shown that the matrix $\mathbf{H_q}$ satisfies the following two equations:

$$\mathbf{H_q^t B_q H_q = I} \quad \text{and} \quad \mathbf{H_q^t\ A_q\ H_q = D_q}. \tag{20}$$

With the coefficients of the $(p_{\text{out}}+1)\times(p_{\text{out}}+1)$ matrices $\mathbf{B}_q$ and $\mathbf{A}_q$ given by

$$\begin{aligned}
b_{ij}^q &= \int_{\Gamma_q}\rho_q^{i+j-2}f_q(\rho_q)d\sigma_q\\
a_{ij}^q &= \int_{\Gamma_q}\rho_q^{i+j-1}f_q(\rho_q)d\sigma_q
\end{aligned} \tag{21}$$

where f_q is the probability density function (pdf) of the random variable $\rho_q\ (\theta)$ and $\mathbf{D}_q$ is a diagonal matrix with diagonal coefficients d_q^i which are not known *a priori*. We note that the coefficients are the moments of the random variables and the moments up to the order $2p_{\text{out}}-1$ are needed to determine the polynomials of order p_{out}. To find the matrix $\mathbf{H}_q$, a problem can be solved which consists in finding the real numbers (eigenvalues) ρ_i and the vectors (eigenvector) $\mathbf{X}_i$ such that

$$(\mathbf{A}_q - \rho_i\mathbf{B}_q)\mathbf{X}_i = 0. \tag{22}$$

The $p_{\text{out}}+1$ vectors provide the columns of the matrix $\mathbf{H}_q$ (so the coefficients of the polynomials) and the eigenvalues provide the value of the coefficients d_q^i. To calculate the coefficients Σ_m^q [see (17)], we need to express ρ_q as a function of the polynomials h_q^i

$$\rho_q = \sum_{i+1}^{P_{\text{out}}+1} \rho_q^i h_q^i. \tag{23}$$

If the pdf of the random variable $\rho_q\ (\theta)$ has been used as the weighted function to generate classical orthogonal polynomials (i.e., with different orders), $\rho_q\ (\theta)$ would have been equal to a linear combination of the polynomials of zero and first orders. With the double orthogonal polynomials, the random variable is a linear combination of all the polynomials. For all random variables $\rho_q\ (\theta)$, we have calculated double orthogonal polynomials. In the following, we will assume that all these polynomials have the same order p_{out}. We will now construct the set of multivariate polynomials $(H_j\ (\theta))_{1\le j\le P_{\text{out}}}$ with $P_{\text{out}} = (p_{\text{out}}+1)^M$ that will be used for the approximation in (15)

$$\begin{aligned} H_j(\theta) &= H_j[\rho_{j1}(\theta)\dots\rho_{jM}(\theta)] \\ &= \prod_{q=1}^{M} h_q^{j_q}[\rho_q(\theta)] = \prod_{q=1}^{M} h_q^{j_q}(\theta) \end{aligned}$$

with

$$j = \sum_{q=1}^{M} (p_{\text{out}}+1)^{q-1}(j_q-1)+1$$

with

$$j_i \in [1, p_{\text{out}}+1] \quad \text{and} \quad i \in [1, M]. \tag{24}$$

Since the random variables $\rho_q\ (\theta) q \in [1, M]$ are assumed to be independent, we can verify the following properties:

$$\begin{aligned} E[H_i(\theta)H_j(\theta)] &= \prod_{q=1}^{M} E\left[h_q^{i_q}(\theta)h_q^{j_q}(\theta)\right] = \delta_{ij} \\ E[\rho_m(\theta)H_i(\theta)H_j(\theta)] &= E\left[\rho_m(\theta)h_m^{i_m}(\theta)h_m^{j_m}(\theta)\right] \\ &\quad \times \prod_{\substack{q=1\\q\neq m}}^{M} E\left[h_q^{i_q}(\theta)h_q^{j_q}(\theta)\right] \\ &= d_m^{i_m}\delta_{ji}. \end{aligned} \tag{25}$$

From these expressions, it can be seen that the multivariate polynomials remain orthogonal. The second property that of the nullity of the expectation of the product of two polynomials with a random variable is also preserved if both are not equal.

To solve the scalar potential formulation, new multivariate double orthogonal polynomials need to be calculated using the approach described above considering the conductivity $\sigma_q\ (\theta)$ instead of the resistivity $\rho_q\ (\theta)$.

IV. Solution of the Stochastic Problem

If we use double orthogonal polynomials to approximate the random dimension, according to the second relation in (25), the matrix $\mathbf{D}_q$ is diagonal (cf., the expression of the coefficients of the matrix d_q^{mj}). If the matrix $\mathbf{D}_d$ is diagonal, solving problem (16) is equivalent to solving P_{out} independent equation systems of the size of the deterministic problem. The jth problem corresponds to a combination of the M-uplet $(j_1, \dots, j_M)$ with j_i an integer belonging to $\{1, \dots p_{\text{out}}+1\}$. The value T_{aj} is the value of the coefficient associated with the edge a for the polynomial $H_j\ (\theta)$. Thus, the solution of the jth problem gives the coefficient of the polynomial $H_j\ (\theta)$ for all edges.

The calculation of the matrix of the jth problem is done as in the deterministic case with a resistivity $\rho\ (x)$ given by (6) where resistivities ρ_q are not random anymore but equal to d_q^{jq}. According to (17), it means that we have to solve P_{out} deterministic problems with a stiffness matrix $\mathbf{S}_j$ given by

$$\mathbf{S}_j = \sum_{q=1}^{M} d_q^{j_q}\mathbf{S_q} \tag{25}$$

and with a source term equal to

$$\begin{aligned} \mathbf{F} &= \sum_{q=1}^{M} e_q^{j_q}\mathbf{F}_q \\ e_q^j &= VE[\rho_q(\theta)H_j(\theta)] \\ &= E\left[\rho_q(\theta)h_q^{jq}(\theta)\right]\prod_{\substack{mi=1\\m\neq q}}^{M} E\left[h_m^{j_m}(\theta)\right] = \rho_q^{j_q}\prod_{\substack{m=1\\m\neq q}}^{M} c_m^{j_m}. \end{aligned} \tag{26}$$

The coefficients ρ_q^{jq} have been introduced in (23) and the coefficients c_m^{jm} are the mean of the random variable $h_m^{jm}\ (\theta)$. A method of calculating the terms ρ_q^{jq} and c_m^{jm} is given in the Appendix. In effect, the stochastic problem can be solved using a deterministic code.

V. Application

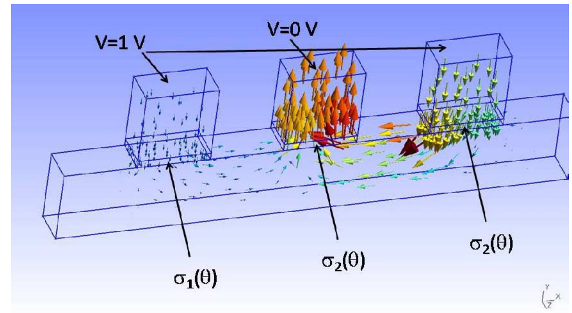

Fig. 1. Description of the device studied and current density distribution obtained for a realization of the random conductivities.

Consider a structure made of four aluminum sections. Three identical sections are affixed on the fourth (main section). We propose to take into account the contact resistances that exist between the upper sections and the main section when they are affixed together. To do so, an intermediate resistive layer is introduced between each two sections, forming the contact. The geometry of the structure and the boundary condition are given in Fig. 1. We calculate the expectation of power for both formulations and for four meshes $(M1, M2, M3, M4)$. We consider an approximation of the first, second, third, and fourth order ($p_{\text{out}} = 1, 2, 3,$ and 4) for the multivariate polynomials $H_i\ (\theta)$ which lead to calculation of $P_{\text{out}} = 8, 27, 64, 225$ "deterministic" problems. The evolution of the power expectation as a function of the number of elements is given in Figs. 2 and 3. A

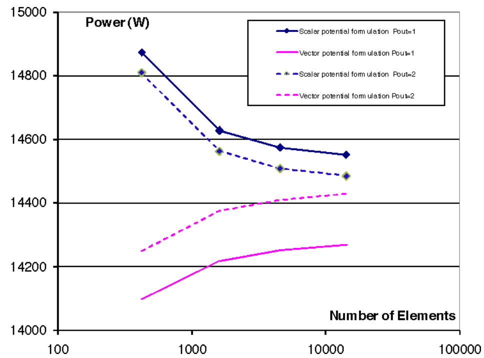

Fig. 2. Evolution of the power expectation for both formulations and for different order of approximation in the stochastic dimension equal to 1 and 2 and different meshes.

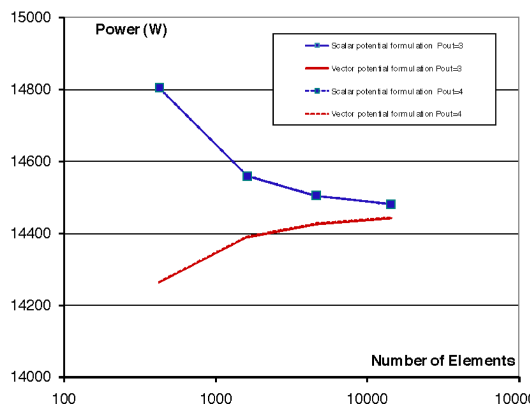

Fig. 3. Evolution of the power expectation for both formulations and for different order of approximation in the stochastic dimension equal to 3 and 4 and different meshes.

power bound can be seen in the stochastic case just as in the deterministic case. In fact, for any combination of conductivities, a deterministic problem can be solved leading to the following power bound:

$$W_\varphi \geq W_{ex} \geq W_T \tag{27}$$

with W_{ex} the exact solution and W_φ and W_T the values of the power given, respectively, by the scalar and the vector potential formulations. Consequently, if we look now at the expectation of the power, we have

$$E(W_\varphi) \geq E(W_{ex}) \geq E(W_T). \tag{28}$$

The difference between the power expectation given by both formulations is an indication of the numerical error. Therefore, the closer the energies are, the more accurate the model. According to that statement, we can see that whatever the order of interpolation, the error decreases with the number of elements. But it can also be seen that up to an order two the accuracy on the power mean does not improve much.

VI. Conclusion

The use of multivariate double orthogonal polynomials to solve a stochastic problem in electrokinetics has been presented. Numerous small linear systems are then solved instead of one huge linear system obtained with the classical SSFEM. The method has been successfully applied to an academic example.

Appendix

Consider the set of polynomials of order $p_{\text{out}} (h_q^j)_{1\leq j\leq p_{\text{out}}+1}$ [the coefficient of the jth polynomial are $(h_q^{ji})_{1\leq j\leq p_{\text{out}}+1}$; see (18)]. We can express the monome x^n $(n \leq p_{\text{out}})$ as a linear combinatison of the previous polynomials

$$x^n = \sum_{j=1}^{p_{\text{out}}+1} y_{qn}^j h_q^j(x). \tag{1.1}$$

To calculate the coefficients $\mathbf{Y}_{qn} = (y_{qn}^j)_{1\leq j\leq p_{\text{out}}+1}$, the system

$$\mathbf{H}_q \mathbf{Y}_{qn} = \mathbf{S}_n \tag{1.2}$$

can be solved, where the jth column of $\mathbf{H}_q$ is the coefficient of the polynomial h_{qj} ranked in increasing order and $\mathbf{S}_n$ the vector with $p_{\text{out}}+1$ components such that all components are equal to zero except the nth component, which is equal to 1. From that, it is easy to determine the coefficients ρ_q^j and c_q^j

$$\begin{aligned}\rho_q^j &= E\left[\sigma_q(\theta) h_q^j(\theta)\right] \\ &= E\left[h_q^j(\theta)\sum_{j=1}^{p_{\text{out}}+1} y_{q1}^j h_q^j(x)\right] = y_{q1}^j \\ c_q^j &= E\left[h_q^j(\theta)\right] \\ &= E\left[h_q^j(\theta)\sum_{j=1}^{p_{\text{out}}+1} y_{q0}^j h_q^j(x)\right] = y_{q0}^j.\end{aligned} \tag{1.3}$$

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