Fast Model Order Reduction Approach to Uncertainty Quantification in Electrokinetics

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Abstract— A novel approach based on Model Order Reduction and Polynomial Chaos Expansion is proposed for uncertainty quantification in electrokinetics due to randomness in material parameters. Such approach is validated by considering a simplified geometry of a typical system for resistance welding. In this situation the Model Order Reduction approach allows to reduce the computational time by about two orders of magnitude with respect to the most efficient approaches based on sparse-grids.

1. INTRODUCTION

The perfect knowledge of material parameters is required in electromagnetic computations. However in many cases some uncertainty must be associated with that knowledge in the modeling process. In order to quantify the uncertainty of the output quantities of interest coming from the lack of knowledge of the input material parameters, the spectral stochastic finite element method, based on Polynomial Chaos Expansion (PCE), can be applied. This method, in both the intrusive and non-intrusive forms [1], allows to dramatically reduce computational time with respect to Monte Carlo (MC) methods. Nevertheless, in many applications computational complexity can still be prohibitively large.

In this paper, uncertainty quantification (UQ) in electrokinetic problems due to randomness in material parameters is considered. For such problems a novel approach based on Model Order Reduction (MOR) is here proposed. MOR was first introduced for accelerating UQ in [2]. Our starting point is a non-intrusive PCE method, in which the PCEs of the variables are estimated from the solutions of the deterministic electrokinetic problems for all values of the random material parameters in a sparse grid. The main idea of the proposed algorithm is that of reducing the number of solutions of such deterministic electrokinetic problems by constructing a parametric reduced order model, which is used to approximate the solution to the deterministic electrokinetic problems. Such parametric reduced order model is tailored to approximate with a chosen accuracy the deterministic elecrokinetic problems for the values of the random material parameters in the chosen sparse grid. The parametric reduced order model is generated in an efficient way by solving a reduced number of deterministic elecrokinetic problems with respect to that in a non-intrusive PCE approach. Moreover the computational cost for the solutions to the deterministic elecrokinetic problems required to construct the parametric reduced order model is optimized by exploiting the relatedness among the solutions to the deterministic electrokinetic problems for different values of the random material parameters.

The proposed MOR approach is then validated by modeling a simplified geometry of a typical system for resistance welding [3]. In this situation the MOR approach allows to reduce the computational time by about two orders of magnitude with respect to that of a standard non-intrusive PCE approach, maintaining the same level of accuracy. The storage requirement of the novel approach is comparable to that of a single deterministic electrokinetic problem. The proposed approach thus seems a novel promising candidate for uncertainty quantification analysis in electrokinetics. The extension of the approach to more general electromagnetic problems seems feasible and is currently under investigation.

2. DETERMINISTIC ELECTROKINETIC FORMULATION

A deterministic electrokinetic problem in the spatial domain Ω is ruled by the equation

$$\nabla \cdot (-\sigma(\mathbf{r}, \mathbf{p}) \nabla \varphi(\mathbf{r}, \mathbf{p})) = 0, \tag{1}$$

in which $\sigma(\mathbf{r}, \mathbf{p})$ is the electric conductivity, function of the position vector $\mathbf{r}$ and of J parameters p_j, with $j = 1, \ldots, J$, forming a vector $\mathbf{p}$. The unknown $\varphi(\mathbf{r}, \mathbf{p})$ is the electric potential, which is a function of both the position vector $\mathbf{r}$ and the parameters vector $\mathbf{p}$. Such electric conductivity

distribution is assumed to be a linear combination of the J parameters p_j, with $j = 1, \ldots, J$, forming vector $\mathbf{p}$, in the form

$$\sigma(\mathbf{r}, \mathbf{p}) = \sigma_0(\mathbf{r}) + \sum_{j=1}^{J} \sigma_j(\mathbf{r})\, p_j. \tag{2}$$

Conditions on the boundary $\partial\Omega$, of outward unit vector $\mathbf{n}(\mathbf{r})$, are assumed of mixed Dirichlet's and Neumann's type. Thus, in the part Σ_φ of the boundary $\partial\Omega$, the electric potential is assigned, so that

$$\varphi(\mathbf{r}, \mathbf{p}) = \varphi_s(\mathbf{r}), \tag{3}$$

while in the remaining part Σ_j of the boundary $\partial\Omega$, the normal component of current density is assigned

$$-\sigma(\mathbf{r}, \mathbf{p}) \frac{\partial \varphi}{\partial n}(\mathbf{r}, \mathbf{p}) = j_s(\mathbf{r}).$$

As it is well known a Finite Element Model (FEM) can be constructed by rewriting the electrokineticks problem in the weak form

$$\int_\Omega \nabla u'(\mathbf{r}) \cdot \sigma(\mathbf{r}, \mathbf{p}) \nabla (u(\mathbf{r}, \mathbf{p}) + \varphi_s(\mathbf{r}))\, d\mathbf{r} + \int_{\Sigma_\varphi} u'(\mathbf{r}) j_s(\mathbf{r})\, d\mathbf{r} = 0. \tag{4}$$

for all functions $u'(\mathbf{r})$, in which $u'(\mathbf{r})$ and $\varphi(\mathbf{r}, \mathbf{p}) = u(\mathbf{r}, \mathbf{p}) + \varphi_s(\mathbf{r})$ belong to the same chosen FEM space X of dimension $|X| = N$. Besides $\varphi_s(\mathbf{r})$ is constructed in X starting from its trace on Σ_φ given by (3); $u(\mathbf{r}, \mathbf{p})$ and $u'(\mathbf{r}, \mathbf{p})$ are assumed to belong to X and to be zero over Σ_φ.

3. STOCHASTIC ELECTROKINETIC FORMULATION

The electric conductivities are now modeled as random variables. Thus in a stochastic analysis the parameters forming vector $\mathbf{p}$ are assumed to be random variables. Applying PCE, $u(\mathbf{r}, \mathbf{p})$ is approximated in the form

$$u(\mathbf{r}, \mathbf{p}) = \sum_{|\boldsymbol{\beta}| \le M} u_{\boldsymbol{\beta}}(\mathbf{r}) \psi_{\boldsymbol{\beta}}(\mathbf{p}), \tag{5}$$

in which $\boldsymbol{\beta}$ are multi-indices of J elements and $\psi_{\boldsymbol{\beta}}(\mathbf{p})$ are polynomials of degrees less than a chosen value M, constituting an orthonormal basis of $Q = \binom{M+J}{J}$ elements, in the probability space of random variables forming vector $\mathbf{p}$. Both intrusive and non-intrusive PCE approaches can be approached to determine (4). In non-intrusive PCE approaches, commonly adopted as the most efficient alternative to Monte Carlo techniques, functions $u_{\boldsymbol{\beta}}(\mathbf{r})$ are reconstructed from the solutions $\varphi(\mathbf{r}, \mathbf{p})$ of the deterministic problems (4) for all values of $\mathbf{p}$ in a proper set $\mathcal{G}$. However, even using sparse-grids [1], the set $\mathcal{G}$ becomes very large when the number J of parameters or the polynomial degree M increases. Thus the number of deterministic problems to be solved also becomes very large.

4. THE MODEL ORDER REDUCTION APPROACH

Hereinafter the alternative Algorithm 1 is proposed which constructs a reduced order model tailored to PCE analysis solving a much smaller number of deterministic problems with respect to the non-intrusive approaches. Moreover the computational cost of the solution to these deterministic problems is much smaller with respect to the non-intrusive approaches, since accurate estimations of the solution to these deterministic problems are derived from the reduced order model solutions taken as starting points in the adopted iterative methods for solving linear systems. The PCE expansion of the solution to the original problem is then obtained from such reduced order model.

In the algorithm, at step 1, the FEM discretization of the electrokinetics deterministic problem (4) is numerically approximated, for each selected value of $\mathbf{p}$. A preconditioned conjugate gradient method is used and the number of iterations is reduced by assuming as initial point the $\hat{\varphi}(\mathbf{r}, \mathbf{p})$ estimation provided by the previously computed compact model. At step 2 an orthonormal basis of

Algorithm 1: MOR-based algorithm

Set $k := 0$ (dimension of the reduced model);
Set $\vartheta := 0$ (norm of the residual);
Set linear space $\mathcal{S}_0 := \emptyset$;
Choose vector $\mathbf{p}$ in $\mathcal{G}$;
Set $\hat{\varphi}(\mathbf{r}, \mathbf{p}) := 0$;
repeat
  Set $k := k + 1$;
1 Solve problem (4) for $\varphi(\mathbf{r}, \mathbf{p})$ using $\hat{\varphi}(\mathbf{r}, \mathbf{p})$ as initial estimation in the iterative technique;
2 Generate an orthonormal basis of the linear space $\mathcal{S}_k$ spanned by $\mathcal{S}_{k-1}$ and $\varphi(\mathbf{r}, \mathbf{p})$;
3 Generate reduced order model $\mathcal{R}_k(\mathbf{p})$, projecting problem $\mathcal{D}$ onto space $\mathcal{S}_k$;
  for all $\mathbf{q} \in \mathcal{G}$ **do**
4 Solve the reduced order model $\mathcal{R}_k(\mathbf{q})$ obtaining $\hat{\varphi}(\mathbf{r}, \mathbf{q})$ as an approximation for $\varphi(\mathbf{r}, \mathbf{q})$;
5 Estimate the approximation residual η;
  if $\eta > \vartheta$ **then**
    Set $\vartheta := \eta$;
6 Set $\mathbf{p} := \mathbf{q}$;
until $\vartheta > \varepsilon$;
7 Determine the PCE expansion of the solution to the reduced order model $\mathcal{R}_k(\mathbf{p})$ and reconstruct the PCE expansion of $\varphi(\mathbf{r}, \mathbf{p})$;

space $\mathcal{S}_k$ is generated, computing a set of functions $v_h(\mathbf{r})$, with $h = 1, \ldots, k$, spanning all functions $u(\mathbf{r}, \mathbf{p})$ computed at step 1 and forming a column vector

$$\boldsymbol{v}(\mathbf{r}) = [v_h(\mathbf{r})].$$

At step 3 the reduced order model $\mathcal{R}_k(\mathbf{p})$ is constructed. This model is obtained from (4) assuming that the X space is substituted by its subspace $\mathcal{S}_k$, spanned by functions $v_h(\mathbf{r})$, with $h = 1, \ldots, k$. In this way the compact model takes the form

$$\left(\hat{\mathbf{S}}_0 + \sum_{j=1}^{J} p_j \hat{\mathbf{S}}_j\right) \hat{\mathbf{x}}(\mathbf{p}) = \left(\hat{\mathbf{R}}_0 + \sum_{j=1}^{n} p_j \hat{\mathbf{R}}_j\right) \tag{6}$$

in which $\hat{\mathbf{S}}_j$, with $j = 1, \ldots, J$, are square matrices of dimension k given by

$$\hat{\mathbf{S}}_j = \left[\int_\Omega \nabla v_h(\mathbf{r}) \cdot \sigma_j(\mathbf{r}) \nabla v_l(\mathbf{r})\, d\mathbf{r}\right], \quad j = 1, \ldots, J,$$

and $\hat{\mathbf{R}}_j$, with $j = 1, \ldots, J$, are column vectors of k rows

$$\hat{\mathbf{R}}_0 = \left[-\int_{\partial\Omega} v_h(\mathbf{r}) j_s(\mathbf{r}) - \int_\Omega \nabla v_h(\mathbf{r}) \cdot \sigma_0(\mathbf{r}) \nabla \varphi_s(\mathbf{r})\, d\mathbf{r}\right],$$
$$\hat{\mathbf{R}}_j = \left[-\int_\Omega \nabla v_h(\mathbf{r}) \cdot \sigma_j(\mathbf{r}) \nabla \varphi_s(\mathbf{r})\, d\mathbf{r}\right], \quad j = 1, \ldots, J.$$

Vector $\hat{\mathbf{x}}(\mathbf{p})$ allows to approximate the solution $u(\mathbf{r}, \mathbf{p})$ to (4) as (step 4)

$$\hat{u}(\mathbf{r}, \mathbf{p}) = \sum_{h=1}^{k} v_h(\mathbf{r}) \hat{x}_h(\mathbf{p}) = \boldsymbol{v}^T(\mathbf{r}) \hat{\mathbf{x}}. \tag{7}$$

At step 5, η represents the residual when $\varphi(\mathbf{r}, \mathbf{q})$ is substituted by $\hat{\varphi}(\mathbf{r}, \mathbf{q}) = \hat{u}(\mathbf{r}, \mathbf{p}) + \varphi_s(\mathbf{r})$ in (4). At step 6, the value of $\mathbf{q}$ in $\mathcal{G}$ maximizing the value of η becomes the candidate $\mathbf{p}$ for solving the deterministic problem (4) at next step 1. At step 7, an intrusive PCE approach is applied to the reduced order model $\mathcal{R}_k$. Thus $\hat{\mathbf{x}}(\mathbf{p})$ is approximated by its PCE

$$\hat{\mathbf{x}}(\mathbf{p}) = \sum_{|\boldsymbol{\beta}| \leq M} \hat{\mathbf{x}}_{\boldsymbol{\beta}} \psi_{\boldsymbol{\beta}}(\mathbf{p}). \tag{8}$$

Substituting this expansion into (6), multiplying then (6) by $\psi_{\boldsymbol{\alpha}}(\mathbf{p})$, with $|\boldsymbol{\alpha}| \leq M$, and applying the expected value operator $\mathbf{E}[\cdot]$, it results in

$$\left(\mathbf{I}_N \otimes \hat{\mathbf{S}}_0 + \sum_{j=1}^{J} \mathbf{P}_j \otimes \hat{\mathbf{S}}_j\right) \hat{\mathbf{X}} = \left(\mathbf{I}_N \otimes \hat{\mathbf{R}}_0 + \sum_{j=1}^{N} \mathbf{P}_j \otimes \hat{\mathbf{R}}_j\right),$$

in which $\hat{\mathbf{X}} = [\hat{\mathbf{x}}_{\boldsymbol{\alpha}}]$ is a column vector with kQ columns and

$$\mathbf{P}_j = [\mathbf{E}[p_j \psi_{\boldsymbol{\alpha}}(\mathbf{p}) \psi_{\boldsymbol{\beta}}(\mathbf{p})]]$$

are square matrices of order Q. This linear system of equations has reduced dimensions with respect to an intrusive PCE approach, so that it can be solved at negligible cost. From the PCE expansion of $\hat{\mathbf{x}}(\mathbf{p})$, the PCE expansion of $\hat{u}(\mathbf{r}, \mathbf{p})$ approximating the PCE of $u(\mathbf{r}, \mathbf{p})$ is straightforwardly obtained as

$$\hat{u}_{\boldsymbol{\alpha}}(\mathbf{r}, \mathbf{p}) = \sum_{|\boldsymbol{\beta}| \leq M} \boldsymbol{v}^T(\mathbf{r}) \hat{\mathbf{x}}_{\boldsymbol{\beta}} \psi_{\boldsymbol{\beta}}(\mathbf{p}). \tag{9}$$

5. NUMERICAL RESULTS

The 3D problem shown in Fig. 1 is considered [3]. The geometry describes three aluminum electrodes over a conductive aluminum substrate. Three contact resistances are modeled by three statistically independent conductivities σ_1, σ_2, σ_3, with uniformly distributed probability density functions in the range 1.41 MS/m–11.3 MS/m.

The conductive region without the surrounding air region is discretized. Homogeneous Neumann's boundary conditions are used everywhere, with the exception of the three electrodes at which Dirichlet's boundary conditions are used, as indicated in Fig. 1. A set of primal tetrahedral grids is generated. Among these a tetrahedral mesh with about $N = 16,000$ nodes is chosen whose

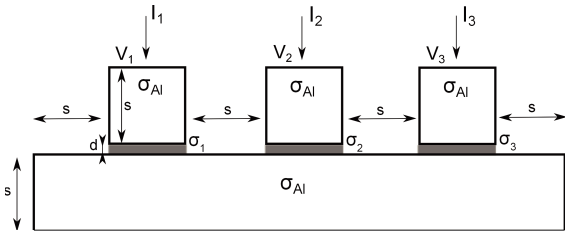

Figure 1: 2D section of the considered example, the depth being equal to s, with $s = 10\,\text{mm}$ and $d = 1\,\text{mm}$.

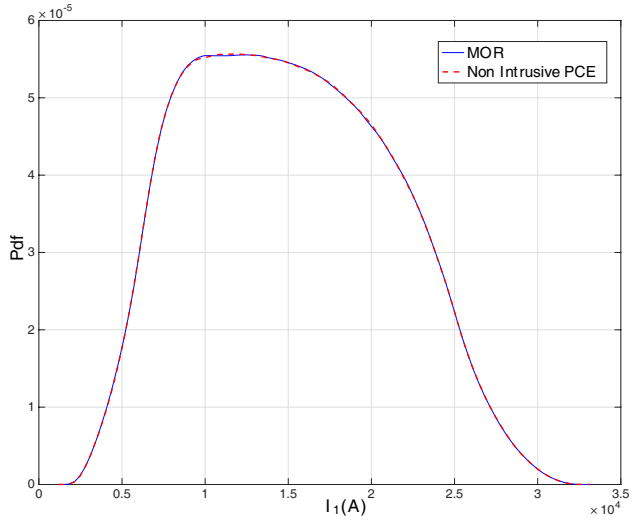

Figure 2: Probability density function of the current I_1.

further refining introduces variations in the potential distribution lesser that 1% in the energy norm. A first order FEM disretization is performed over such mesh.

The PCE of the electric current I_1 is estimated in the situation in which $V_1 = V_3 = 1$ and $V_2 = 0$. A PCE order $M = 7$ is assumed and a Gauss-Legendre sparse grid $\mathcal{G}$ of dimension $|\mathcal{G}| = 681$ is used. With these choices the non-intrusive PCE approach requires the solution of 681 sistems of equations. By applying a preconditioned conjugate gradient algorithm this requires about 167.7 s on a 2.3 Ghz Intel Core i7. Instead the application of Algorithm 1 allows to approximate the solution of the problem with a 0.01% accuracy in $k = 5$ steps and in about 1.5 s, with about two orders of magnitude improvement in computational time.

In Fig. 2, the probability density function (Pdf) of the current I_1 computed by Algorithm 1 is compared to the solution computed by the non-intrusive PCE approach, showing excellent agreement. The tiny difference visible in the two pdfs of Fig. 2 is not due to the difference in the MOR and non intrusive PCE solutions but to the approach used to estimate the probability density function starting from the PCE of I_1. In Fig. 3, the error in the approximation of the PCE of the spatial distribution of the electric potential is shown as a function of the step number k in Algorithm 1, showing a practically exponential decay with respect to k.

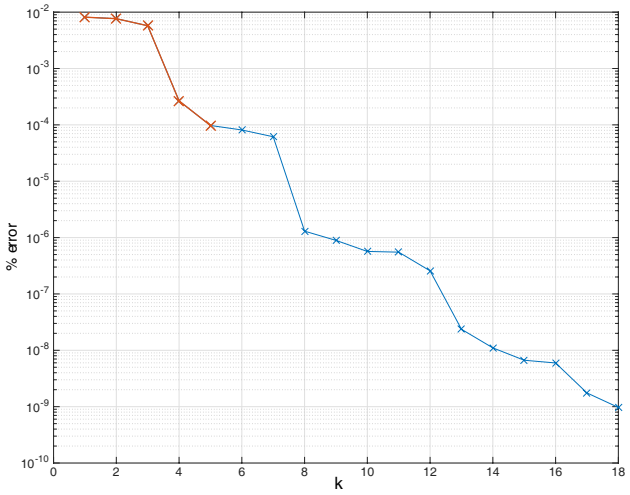

Figure 3: Relative error in the energy norm of the PCE of the electric potential as a function of the step number k of Algorithm 1. The red line shows the iteration steps performed for getting a 0.01% accuracy.

6. CONCLUSION

In this paper a novel approach based on MOR has been proposed for uncertainty quantification problems due to random material parameters in electrokinetics. The proposed MOR approach has been validated by considering a simplified geometry of a typical system for resistance welding. In this situation the novel approach allowed to reduce the computational time by about two orders of magnitutude with respect to that of standard non-intrusive PCE approach, maintaining the same level of accuracy.

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