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A stochastic collocation method combined with a reduced basis method to compute uncertainties in numerical dosimetry

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A reduced basis method is introduced to deal with a stochastic problem in a numerical dosimetry application in which the field solutions are computed using an iterative solver. More precisely, the computations already performed are used to build an initial guess for the iterative solver. It is shown that this approach significantly reduces the computational cost.

Index Terms—Finite-element methods, numerical analysis, dosimetry.

I. INTRODUCTION

The lack of knowledge on the electric parameters of tissues raises an issue in computational electromagnetic applications such as numerical dosimetry [1]. The Stochastic Collocation Method (SCM) is an “attractive” technique to deal with this kind of problem because existing deterministic solvers can be readily applied like in the Monte Carlo sampling [2]. We use the SCM coupled with a Smolyak Adaptive Algorithm (SAA) [3] which enables to build the solution gradually by an adaptive choice for the realizations of the input random parameters (these realizations will be called the “collocation points”). Every step of the SAA involves several collocation points, and each of them requires a deterministic computation that can be numerically expensive in realistic applications. When the deterministic computations are performed sequentially using an iterative solver, the computations already performed could be used to reduce the computational cost. The authors of [4] proposed to choose as the initial guess for the iterative solver the previous computed solution for which the collocation point is “close” to the next considered point. Here, we propose to compute an initial guess with the Reduced Basis Method (RBM); this practical aspect is not studied in the RBM papers [5,6]. “Similar” ideas have already been used in a transient implicit time integration process [7] but their approach was not dedicated to systems with varying parameters. Moreover, we couple the RBM with an A Posteriori Error Indicator (APEI) to choose the next collocation point.

First we review some aspects of the RBM; for complementary details see also [5]. Then, numerical experiments on a wave equation problem show that the computational cost of the solver can be significantly reduced. Finally, we point out some limitations due to the nature of the SAA.

II. REDUCED BASIS METHOD

A. Finite element approximation

We are interested in solving the time-harmonic Maxwell equations in a 3D domain $\Omega = \bigcup_{k=1}^p \Omega_k$, where the Ω_k are non-overlapping subdomains. Each subdomain Ω_k is characterized by a constant electric parameter $\tilde{\epsilon}^k = \epsilon_0 \epsilon_r^k + \sigma^k / j\omega$, where ϵ_0 denotes the vacuum permittivity, ω the angular frequency, ϵ_r^k the relative permittivity and σ^k the conductivity of the subdomain Ω_k .

In the stochastic context, the parameters ϵ_r^k and σ^k are considered as independent random variables. For a given realization of these random variables, the weak formulation to compute the electric field \vec{E} on a conforming Finite Element (FE) space X_h can be written:

$$a(\vec{E}(\tilde{\epsilon}), \vec{E}', \tilde{\epsilon}) = f(\vec{E}') \quad \forall \vec{E}' \in X_h, \tilde{\epsilon} = (\tilde{\epsilon}^1, \dots, \tilde{\epsilon}^p), \quad (1)$$

$$\begin{aligned} \text{with } a(\vec{E}, \vec{E}', \tilde{\epsilon}) &= a_0(\vec{E}, \vec{E}') - \sum_{k=1}^p \omega^2 \mu_0 \tilde{\epsilon}^k a_k(\vec{E}, \vec{E}'), \\ a_0(\vec{E}, \vec{E}') &= \int_{\Omega} \nabla \times \vec{E} \cdot \overline{\nabla \times \vec{E}'} dx + BT, \\ a_k(\vec{E}, \vec{E}') &= \int_{\Omega_k} \vec{E} \cdot \overline{\vec{E}'} \quad \text{for } 1 \leq k \leq p, \\ \text{and } f(\vec{E}') &= -j\omega \mu_0 \int_{\Omega} \vec{J}_s \cdot \overline{\vec{E}'} \end{aligned}$$

$\nabla \times$ denotes the curl operator, μ_0 the vacuum permeability, \vec{J}_s the electric current source, and BT the boundary term.

The solution of (1) leads to a large sparse linear system:

$$(A_0 - \omega^2 \mu_0 \sum_{k=1}^p \tilde{\epsilon}^k A_k) E(\tilde{\epsilon}) = F, \quad (2)$$

where A_k and F denote the matrix representation of the sesquilinear forms a_k and semilinear form f in the standard basis of X_h , denoted here by $\{\vec{E}'_i; i = 1 \text{ to } n\}$.

Since they do not depend on $\tilde{\epsilon}$, we can pre-assemble in an offline procedure the corresponding values:

$$\begin{aligned} A_{kij} &= a_k(\vec{E}'_j, \vec{E}'_i) \quad \text{for } i, j = 1 \text{ to } n \text{ and } k = 0 \text{ to } p, \\ F_i &= f(\vec{E}'_i) \quad \text{for } i = 1 \text{ to } n. \end{aligned}$$

Thus the matrices $(A_k)_{0 \leq k \leq p}$ and F do not require any calculation when we change the values of $\tilde{\epsilon}$.

In part III, a 3D dosimetry problem with a human head that involves several million unknowns is studied. Consequently the solution of the linear system (2) is computed using an iterative solver. In order to make a smart choice of its initial guess, we propose to build a Reduced Basis from the computed solutions obtained with the previous values of $\tilde{\epsilon}$.

B. Reduced basis approximation

Suppose that the problem (1) has been solved for M different values of the parameters $\tilde{\epsilon}$. In the reduced basis formulation, the local FE space X_h in problem (1) is substituted by a space of functions $X_b \subset X_h$ spanned by the M known solutions. The reduced basis formulation is then:

$$a(\vec{E}_b(\tilde{\epsilon}), \vec{E}', \tilde{\epsilon}) = f(\vec{E}') \quad \forall \vec{E}' \in X_b. \quad (3)$$

For the purpose of well-conditioned systems, a modified Gram-Schmidt process depending on the tolerance α for the residual norm in the iterative solver is used to obtain an orthonormal basis $\{\tilde{\xi}_i; i = 1 \text{ to } N\}$ of X_b with $N \leq M$. Usually, the space X_b has a much smaller dimension than the dimension of X_h ($N \ll n$).

Then, the solution of (3) leads to a linear system

$$(B_0 - \omega^2 \mu_0 \sum_{k=1}^p \tilde{\epsilon}^k B_k) E_b(\tilde{\epsilon}) = F_b, \quad (4)$$

where B_k and F_b denote the matrix representation of the sesquilinear forms a_k and semilinear form f in the basis $\{\tilde{\xi}_i; i = 1 \text{ to } N\}$. This ‘‘small’’ system is solved by Gaussian elimination.

In order to reduce the number of iterations for solving problem (1), we choose as the initial guess the solution to problem (3). Its expression in X_h is given by the vector $WE_b(\tilde{\epsilon})$ where $E_b(\tilde{\epsilon})$ is the solution to the linear system (4) and W is the matrix (n, N) whose column W^j contains the components of $\tilde{\xi}_j \in X_b$ in the FE basis $\{\vec{E}_i'; i = 1 \text{ to } n\}$.

It is advantageous in terms of computational cost to calculate the matrices B_k and the vector F_b by using the relations $B_k = \bar{W}^t A_k W$, $k = 0 \text{ to } p$, $F_b = \bar{W}^t F$, where \bar{W}^t is the conjugate transpose of W . Each addition of an element in the reduced basis only requires the calculation of one new line and one new column for B_k and one new scalar for F_b . Note that once the matrices B_k , $k = 0 \text{ to } p$ and the vector F_b are computed, the cost to build the matrix $B_0 - \omega^2 \mu_0 \sum_{k=1}^p \tilde{\epsilon}^k B_k$ and to solve the linear system (4) becomes independent of n (it only depends on p and N).

C. A posteriori error indicator APEI

Every step of the SAA involves a set of collocation points Σ that have to be calculated. An APEI is introduced to order the set Σ as usually done in the RBM [6]. Problem (4) is first solved for the different values of $\tilde{\epsilon}$ corresponding to the collocation points belonging to Σ . An error indicator is then defined by using the residual norm of the linear system (2):

$$\eta(\tilde{\epsilon}) = \|A(\tilde{\epsilon})WE_b(\tilde{\epsilon}) - F\|^2 \quad \forall \tilde{\epsilon} \in \Sigma, \quad (5)$$

with $A(\tilde{\epsilon}) = A_0 - \omega^2 \mu_0 \sum_{k=1}^p \tilde{\epsilon}^k A_k$, and $\|\cdot\|$ is the euclidian norm. In a similar way to the construction of (4), we pre-compute in an offline procedure the quantities related to this residual:

$$\begin{aligned} & \overline{(A_k W^j)^t} A_{k'} W^j, \quad k, k' = 1 \text{ to } p, \quad i, j = 1 \text{ to } N, \\ & \overline{(A_k W^j)^t} F, \quad k = 1 \text{ to } p, \quad i = 1 \text{ to } N. \end{aligned}$$

Then, we choose $\tilde{\epsilon}_m = \operatorname{argmax}_{\tilde{\epsilon} \in \Sigma} (\eta(\tilde{\epsilon}))$ as the next collocation point for which system (2) has to be solved. This approach is described in Algorithm I for l steps of the SAA.

ALGORITHM I
CONSTRUCTION OF THE REDUCED BASIS AND USE OF THE APEI

```

/* Note that the first step of the SAA generates a single collocation point */
 $\tilde{\epsilon}_1 \leftarrow$  the first step of the SAA.
solve  $A(\tilde{\epsilon}_1)E = F$  with the iterative solver initialized by 0.
 $W^1 \leftarrow \frac{E}{\|E\|}$ 
for  $k = 0$  to  $p$ 
   $B_k = \bar{W}^t A_k W$ 
end
 $F_b = \bar{W}^t F$ 
 $N \leftarrow 2$ 
for  $i = 2$  to  $l$ 
   $\Sigma \leftarrow$  the  $i^{\text{th}}$  step of SAA
  while  $\Sigma \neq \emptyset$ 
    for  $\tilde{\epsilon} \in \Sigma$ 
       $E_b(\tilde{\epsilon}) = (B_0 - \omega^2 \mu_0 \sum_{k=1}^p \tilde{\epsilon}^k B_k)^{-1} F_b$ 
       $\eta(\tilde{\epsilon}) = \|A(\tilde{\epsilon})WE_b(\tilde{\epsilon}) - F\|^2$ 
    end
     $\tilde{\epsilon}^* = \operatorname{argmax}_{\tilde{\epsilon} \in \Sigma} \eta(\tilde{\epsilon})$ 
     $\Sigma \leftarrow \Sigma - \{\tilde{\epsilon}^*\}$ 
    solve  $A(\tilde{\epsilon}^*)E = F$  with the iterative solver initialized by  $WE_b(\tilde{\epsilon}^*)$ .
    /* the modified Gram-Schmidt process */
    if  $\eta(\tilde{\epsilon}^*) > \alpha$ 
       $W^N \leftarrow E$ 
      for  $j = 1$  to  $N - 1$ 
         $W^N \leftarrow W^N - (\bar{W}^N)^t W^j) W^j$ 
      end
       $W^N \leftarrow \frac{W^N}{\|W^N\|}$ 
      for  $k = 0$  to  $p$ 
        compute one new line and one new column in  $B_k$ .
      end
      compute one new scalar in  $F_b$ .
       $N \leftarrow N + 1$ 
    end
  end
end

```

D. RBM cost

The computational cost is evaluated by the number of Arithmetic Operations (AO). Considering a Reduced Basis of dimension N , the computational cost to obtain the initial guess $WE_b(\tilde{\epsilon})$ concerns the building of the linear system (4) that depends in one hand on the previous solutions expressed in the FE basis of dimension n and in the other hand on the solving of this system of dimension $N \times N$. Without using the APEI, the cost C_{RBM} can be estimated as follows:

$$C_{\text{RBM}} \leq pN^4 - 2pN^3 + 9nN^2 + 6CnN + 4n, \quad (6)$$

where C is the maximum non-zero elements in any line of the matrices $(A_k)_{0 \leq k \leq p}$.

Using the APEI, the computational cost to determine $\tilde{\epsilon}_m$ grows with the evaluation of the residual (5) for all collocation points belonging to Σ . Considering a set Σ of N points, the cost C_{APEI} can be estimated as follows:

$$C_{\text{APEI}} \leq (p+1)^2 N^4 + (2p^2 + 5p + 3)N^3 + (2n + 2(p+2)^2)N^2 + (2n + (p+2)^2)N + 2n. \quad (7)$$

Furthermore, the cost in solving (2) with the iterative solver initialized by 0 depends on the number of iterations made by the iterative solver. One have to keep in mind that one iteration to solve a problem of dimension n costs $2Tn$ [8,9], where T is constant that depends mostly on the preconditioning. In the application proposed in part III, we focus our attention in the number of iterations saved by the RBM with and without the APEI.

III. APPLICATION TO A DOSIMETRY PROBLEM

The dosimetry problem studied in this paper concerns the exposition of the Visible Human head to the electromagnetic radiation of a mobile phone as described in [10]. The mobile phone is formed by a monopole antenna and a chassis embedded in plastic, with the excitation point at the base of the antenna. The model of the Visible Human head is constituted of four biological tissues: the brain, the cerebro spinal fluid, the skull and the skin.

As introduced in Section II-A, the problem is solved using the FE method applied to the time-harmonic Maxwell equation. The mesh for the problem considered here is illustrated in Fig. 1. Using the lowest order edge elements in the discretization, the numerical problem involves 1.9 million unknowns. For this problem, the solution of (2) is computed using the Conjugate Orthogonal Conjugate Gradient (COCG) [8] with a potential projection preconditioning technique [9]. The COCG is stopped when the residual norm converges to the desired tolerance $\alpha = 10^{-6}$. We do not focus our attention to evaluate the total numerical error (the error owing the numerical model and the iterative solver).

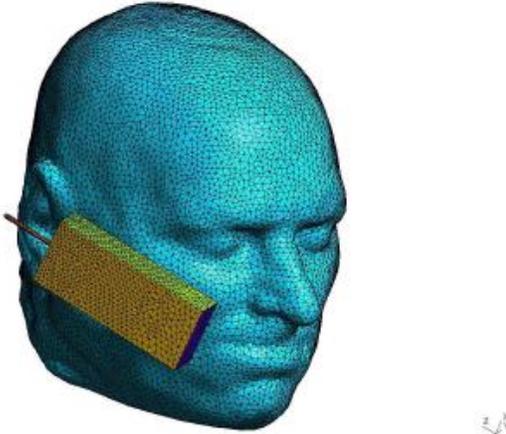


Fig. 1. Mesh of the Visible Human head with the mobile phone.

The quantity of interest in electromagnetic dosimetry is the SAR that measures the quantity of electromagnetic power absorbed by 1 kg of tissue:

$$\text{SAR} = \frac{1}{2} \frac{\sigma |E|^2}{\rho} \text{ (W/Kg)}, \quad (8)$$

where $|E|$ is the amplitude of the electric field and ρ the volumic mass in the considered tissue.

We consider that the relative permittivity and conductivity of the 4 tissues are random variables with uniform laws:

$$\epsilon_r^i \sim U(\epsilon_{r_{\min}}^i, \epsilon_{r_{\max}}^i), \text{ and } \sigma^i \sim U(\sigma_{\min}^i, \sigma_{\max}^i) \quad 1 \leq i \leq 4.$$

More precisely, uniform laws have been chosen with a mean value equal to the value referred in the well-known Gabriel database [11] and with a range of variation of $\pm 10\%$ around the mean value.

To test the efficiency of the RBM, 4 strategies to choose the initial guess in the COCG are tested:

- (i) the zero vector,
- (ii) the nearest previous solution following a distance which is defined in function of the input parameters as in [4]:

$$d(\tilde{\epsilon}_s, \tilde{\epsilon}_t) = \sum_{i=1}^4 \frac{(\epsilon_{r_s}^i - \epsilon_{r_t}^i)^2}{(\epsilon_{r_{\max}}^i - \epsilon_{r_{\min}}^i)^2} + \sum_{i=1}^4 \frac{(\sigma_s^i - \sigma_t^i)^2}{(\sigma_{\max}^i - \sigma_{\min}^i)^2},$$

where $\tilde{\epsilon}_s, \tilde{\epsilon}_t$ are two realizations of $\tilde{\epsilon}$, ϵ_{\min}^i and ϵ_{\max}^i respectively denote the minimum and maximum values of the variable ϵ .

- (iii) the reduced basis approximation without using APEI,
- (iv) the reduced basis approximation by using APEI.

Strategy (ii) is based on the search of the minimum distance for the input parameters of the previous solution in order to choose the previous solution that will be considered as the initial guess for the current computation. In strategy (iv), a residual is computed and it gives an indicator of the error (it can be seen as a distance) between the initial guess built with the RBM and the exact solution. This last strategy is on the contrary based on the search of the maximum of this distance in order to improve the efficiency of the RBM.

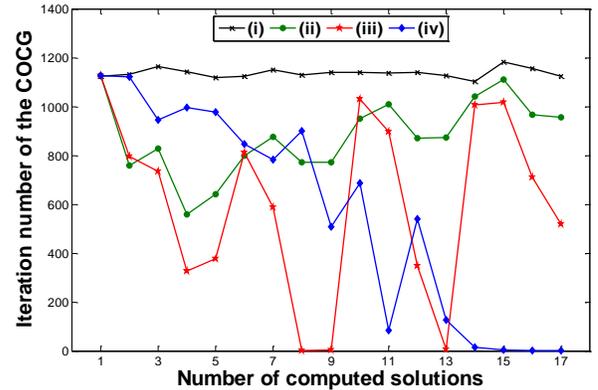


Fig. 2. Iteration number of the solver vs. the number of computed solutions

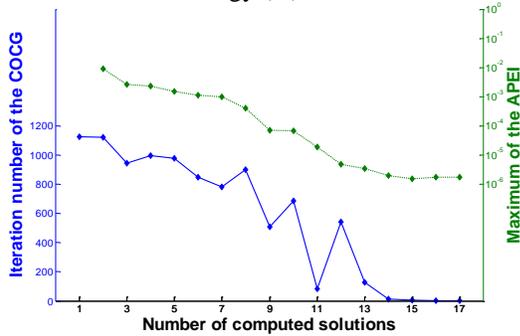
The efficiency of each approach is evaluated by a convergence study of the COCG in computing the 17 collocation points generated by the two first steps of the SAA (two step of SAA are enough to reach an error of 10^{-2} on the variance of the SAR). Results are reported in Fig. 2: the strategies using the RBM approximation need less iterations than (i) and (ii). The total number of the iterations to solve the 17 linear systems (2) is: (i) 19333, (ii) 14912, (iii) 10304, and (iv) 9665 iterations.

Strategies (iii) and (iv) seem to be the most attractive strategies since they save the more iterations. However one has to take into account the computational cost to build the RBM and the APEI. Based on the evaluated costs given in part II-D, Table I synthesizes the real cost of each strategy. It appears that strategies (iii) and (iv) remain more attractive than strategy (ii). Strategy (iv) save more computational cost compared to strategy (iii).

TABLE I

COMPARISON BETWEEN THE COST SAVED IN THE DIFFERENT STRATEGIES			
Strategies	(ii)	(iii)	(iv)
Cost using formulas (6) and (7) with $C = 19$, $p = 4$, $n = 1.9e+6$ and $N = 16$ (AO)	small	7.8e+9	8.9e+9
Number of iterations using the solver	14912	10304	9665
Number of iterations saved compared to strategy (i)	4421	9029	9668
Cost for the iterations saved with $T = 1$ (AO)	1.7e+10	3.4e+10	3.7e+10
Cost saved = line 4 – line 1(AO)	1.7e+10	2.6e+10	2.8e+10

In agreement with the construction of the APEI, Fig. 3 shows that the value of the maximum of the APEI decreases monotonically, and that its trend is nearly the same for the number of iterations in strategy (iv).

Fig. 3. Evolution study of $\max_{\xi \in \Sigma}(\eta(\xi))$

The interest of strategy (iv) appears much more if one goes further in the SAA. Fig. 4 gives the results for ten steps of the SAA (it gives an error of 10^{-6} on the variance of the SAR). The total number of the iterations to solve the 161 linear systems (2) is: (iii) 24637, and (iv) 22916 iterations. But in this case, Fig. 5 shows that the APEI does not decrease monotonically: at each step of SAA it appears an increase of the residual indicator. Actually, the APEI is in conflict with the variance indicator of the SAA [3].

In a last numerical experience called strategy (v), we apply Algorithm I where l is equal to 2 and Σ contains the 160 collocation points obtained from strategy (iii) after ten steps of the SAA. It is fictional but will highlight the interest of the APEI. The total number of iterations to solve the 161 linear systems (2) is: 22205 iterations. The value of the maximum of the APEI decreases monotonically on the 160 points (see Fig. 4 and 5).

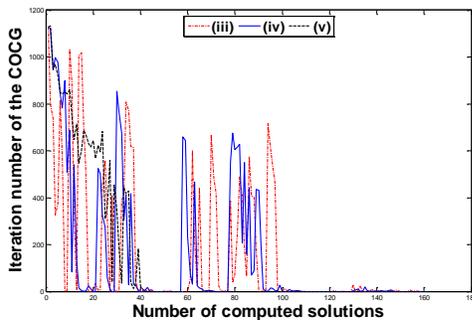
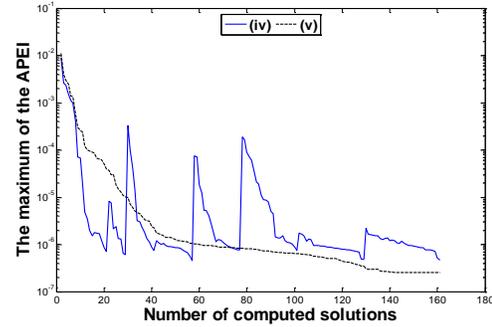


Fig. 4. Iteration number of the solver vs. the number of computed solutions

Fig. 5. Evolution study of $\max_{\xi \in \Sigma}(\eta(\xi))$

IV. CONCLUSION

A stochastic collocation method combined with a reduced basis method has been proposed to study the variability in a 3D dosimetry problem. In the usual stochastic approach, the deterministic calculations are performed separately at the different collocation points without using previous computations. In order to save time in solving the different deterministic problems, it has been proposed to use a RBM without losing the accuracy. This method is efficient because it reduces the number of iterations of the iterative solver; however the adaptivity of the SAA seems in conflict with the APEI. Therefore, it is intended to replace the SAA by a statistical method like the Latin hypercube sampling.

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