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

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Abstract — 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 reduces significantly the computational cost with the same accuracy.

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 here the "collocations 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 numerical 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). Moreover, the RBM is coupled with an A Posteriori Error Indicator (APEI) to choose the next collocation point.

First we review some aspects of the RBM, see also [5]. Numerical experiments on a wave equation problem show that the computational cost of the solver can be significantly reduced.

II. REDUCED BASIS METHOD

A. Finite element approximation

We are interested to solve the wave equation for the electric field E in a domain $\Omega = \bigcup_{i=1}^{p} \Omega_i$, where the Ω_i are non-overlapping subdomains. Each subdomain Ω_i is characterized by a constant electric parameter $\tilde{\varepsilon}^i = \varepsilon_0 \varepsilon_r^i + \sigma^i / j\omega$, where ε_0 denotes the vacuum permittivity, ε_r^i the relative permittivity, σ^i the conductivity, and ω the angular frequency.

In the stochastic context, the parameters ε_r^i and σ^i are considered as independent random variables. For a given realization of these random variables, the weak formulation on a conforming Finite Element (FE) space X_h can be written:

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

with $a(E, E', \tilde{\varepsilon}) = a_1(E, E') - \sum_{i=1}^{p} \omega^2 \mu_0 \tilde{\varepsilon}^i \, a_2^i(E, E') + BT,$

$a_1(E, E') = \int_\Omega \nabla \times E \,.\, \nabla \times E' dx,$

$a_2^i(E, E') = \int_{\Omega_i} E \,.\, E' dx \quad 1 \le i \le p,$

and $f(E') = -j\omega\mu_0 \int_\Omega J_s . E' \, dx.$

$\nabla \times$ denotes the curl operator, . the canonical inner product, μ_0 the vacuum permeability, J_s the electric current source, and BT the boundary term. The solution of (1) leads to a large sparse linear system:

$$A(\tilde{\varepsilon}) \, E = F. \quad (2)$$

For example, a 3D dosimetry problem in a human head [1] involves several million unknowns. Thus, we compute the solution using an iterative solver.

B. Reduced basis approximation

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

$$a(E_{BR}(\tilde{\varepsilon}), E', \tilde{\varepsilon}) = f(E') \quad \forall E' \in X_{BR}. \quad (3)$$

In order to reduce the number of iterations for solving (2), we choose as the initial guess the solution of (3).

Usually, the space X_{BR} has a much smaller dimension than the dimension n of X_h (N is between 10 and 100).

Moreover, the bilinear form a given in (1) is decomposed into forms which are independent of the parameter $\tilde{\varepsilon}$. Thus, given $X_{BR} = \text{span}\{E_h(\tilde{\varepsilon}_1), \dots, E_h(\tilde{\varepsilon}_N)\}$, we can pre-assemble in an offline procedure the corresponding matrices:

$$A_{1_{j,k}} = a_1\left(E_h(\tilde{\varepsilon}_j), E_h(\tilde{\varepsilon}_k)\right) \quad 1 \le j, k \le N, \quad (4)$$

$$A^i_{2_{j,k}} = a_2^i\left(E_h(\tilde{\varepsilon}_j), E_h(\tilde{\varepsilon}_k)\right) \quad 1 \le j, k \le N, 1 \le i \le p.$$

Note that this assembling depends on n, but once the matrices are assembled the computational cost for the solution of (3) is independent of n.

C. A posteriori error indicator

Every step of the SAA involves a set of collocation points Σ. An APEI is introduced to order the set Σ as usually done in the RBM [6]. Our error indicator is defined by using the residual of the linear system (2):

$$\eta(\tilde{\varepsilon}) = \| \, A(\tilde{\varepsilon}) \widetilde{E}_{BR}(\tilde{\varepsilon}) - F \, \| \quad \forall \tilde{\varepsilon} \in \Sigma,$$

where $\widetilde{E}_{BR}(\tilde{\varepsilon})$ represents the projection of $E_{BR}(\tilde{\varepsilon})$ into X_h, and $\|.\|$ is the euclidian norm. In a similar way to (4), we pre-compute in an offline procedure the quantities related to

this residual. Then, we choose $\tilde{\varepsilon}_m = \text{argmax}_{\tilde{\varepsilon}\in\Sigma}(\eta(\tilde{\varepsilon}))$ as the next collocation point for which system (2) has to be solved. This approach is described in Algorithm A1:

Given X_{BR} *and* Σ.
for i = 1,…, size(Σ)
  for each $\tilde{\varepsilon} \in \Sigma$ do
    Compute $E_{BR}(\tilde{\varepsilon})$ solution of (3)
    $\eta(\tilde{\varepsilon}) = \| A(\tilde{\varepsilon})\widetilde{E}_{BR}(\tilde{\varepsilon}) - F \|$
  end
  $\tilde{\varepsilon}_m = \text{argmax}_{\tilde{\varepsilon}\in\Sigma}(\eta(\tilde{\varepsilon}))$
  Solve (2) with $\tilde{\varepsilon}_m$ and $\widetilde{E}_{BR}(\tilde{\varepsilon}_m)$ as the initial guess
  $X_{BR} \longleftarrow \text{span}(X_{BR}, E(\tilde{\varepsilon}_m))$
  $\Sigma \longleftarrow \Sigma - \{\tilde{\varepsilon}_m\}$
end

Algorithm A1: use of the APEI

III. DOSIMETRY PROBLEM

The example concerns a 2D problem of hyperthermia where an electromagnetic wave illuminates a tumor in a patient (see Fig. 1). We consider that the relative permittivity and conductivity of 4 tissues are random variables with uniform laws:

$\varepsilon_r^i \sim U(\varepsilon_{r_{min}}^i, \varepsilon_{r_{max}}^i)$, and $\sigma^i \sim U(\sigma_{min}^i, \sigma_{max}^i)$ $1 \le i \le 4$.

For this problem, the solution of (2) is computed by using the Conjugate Orthogonal Conjugate Gradient (COCG) [7] with a symmetric Gauss-Seidel preconditioner.

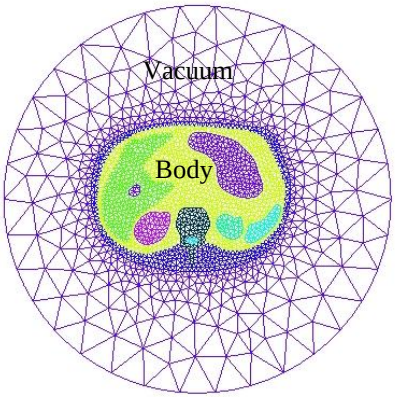

Fig. 1. Mesh for the considered problem

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

(i) the zero vector,
(ii) the nearest previous solution [4] with the following distance:

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

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

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. The relative residual of the COCG is fixed to 10^{-6}. Results are reported in Fig. 2: the strategies using the RBM approximation need less iterations than (i) and (ii). It appears that SCM combined with a RBM reduces the number of iterations. The total number of the iterations to solve the 17 linear systems (2) is: (i) 4284, (ii) 3403, (iii) 2547, and (iv) 2489 iterations.

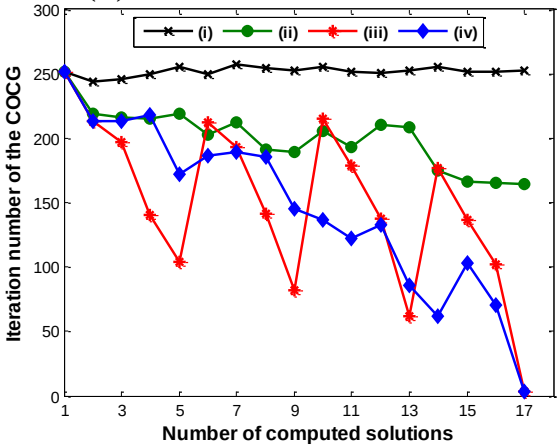

Fig. 2. Iteration number of the solver vs. the number of computed solutions

The value of the maximum of the APEI is reported in Fig. 3: it appears that it decreases monotically. The trend is nearly the same for the number of iteration in strategy (iv) (see Fig. 3).

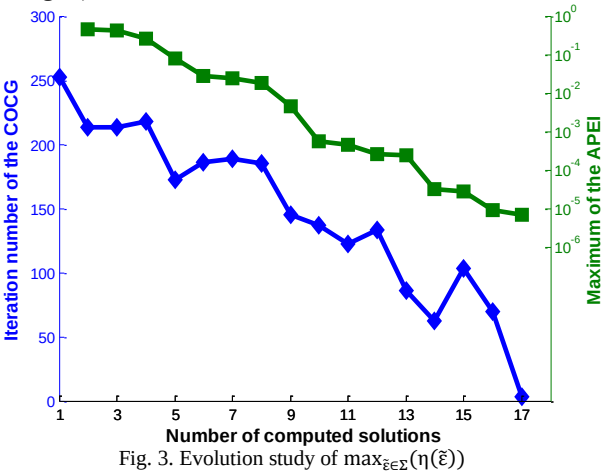

Fig. 3. Evolution study of $\max_{\tilde{\varepsilon}\in\Sigma}(\eta(\tilde{\varepsilon}))$

IV. REFERENCES

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