Fast uncertainty quantification of fields and global quantities

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We introduce a technique for uncertainty quantification of fields and global quantities based on the Guide to the expression of Uncertainty in Measurements (GUM). It is much faster than alternative approaches based on Monte Carlo or polynomial chaos expansion while maintaining good accuracy when the materials uncertainty is moderate. The method is applied to electro-quasistatic (EQS) problems arising in biomedical engineering. A good agreement is found with respect to the Monte Carlo method.

***Index Terms*—finite elements (FEM), finite integration technique (FIT), Guide to the expression of Uncertainty in Measurements (GUM), uncertainty quantification**

THE aim of this paper is to introduce a method for uncertainty quantification in numerical simulations of electromagnetic problems based on the Guide to the expression of Uncertainty in Measurements (GUM) [1]. The proposed method is an instance of the well known design of experiments (DOE) method [2], that, to our knowledge, has never been used for such uncertainty quantification. Its virtues are that it is very fast and straightforward to implement while maintaining good accuracy w.r.t. Monte Carlo or other methods based on polynomial chaos expansion, see [3], [4] when the materials uncertainty is moderate (i.e. at most a few tens per cent).

As an application, we consider state-of-the-art methods for point-of-care diagnostics of the thrombotic risk profile which are based on lab-on-a-chip microfluidic devices where whole blood flows on a surface covered by a thrombogenic substrate [5]. An accurate estimation of thrombus growth is obtained by fusing optical and impedance data [6]. However, the electric properties of blood are not precisely known and vary depending on the individual, the hydration and other physiological parameters. This clearly affects the estimated thrombus growth and it is just an example of application where the impact of material parameters uncertainties is of fundamental importance.

I. Uncertainty quantification based on GUM

The Guide to the expression of Uncertainty in Measurements (GUM) [1] provides the general guidelines, valid for all the fields of applications, to evaluate the uncertainty in measurements. In indirect measurements, the uncertainty is evaluated by means of the law of propagation of uncertainty. If the quantity y is $y = f(x_1, x_2, ..., x_N)$, then the uncertainty on y, $u(y)$, can be expressed as

$$u^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j) = \tag{1}$$

$$= \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i} u(x_i)\right)^2 + \sum_{i=1}^{N}\sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j).$$

In case of uncorrelated input quantities, since $u(x_i, x_j) = 0$ for $i \neq j$, the law of uncertainty propagation reduces to

$$u^2(y) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i} u(x_i)\right)^2. \tag{2}$$

The law of uncertainty propagation leans on two assumptions: the approximation of f with the Taylor's polynomial truncated at first order and the central limit theorem. Truncating the Taylor's polynomial of f at the first order means

$$y = f(x_1, x_2, ..., x_N) \approx \hat{y} + \sum_{i=1}^{N} \frac{\partial f}{\partial x_i}(x_i - \hat{x}_i), \tag{3}$$

where the hat represents the linearization point; this first assumption is valid if the uncertainty of input quantities is small enough to neglect higher orders of nonlinearity of f.

The second assumption (the central limit theorem) assures that the linear combination of a wide number of random variables (each with unknown distribution) tends to a Gaussian behavior, so the uncertainty on y in (1) and (2) has Gaussian Probability Density Function (PDF) with standard deviation $u(y)$, if we consider the square root of central moment of order two for the input quantities $u(x_i)$.

If one or both of these two assumptions are not valid, the uncertainty propagation does not provide an accurate estimation; if none of them is valid, the only way for the GUM is the Monte Carlo method [7], which needs a very long computational time. If only the first assumption is valid, i.e. that the number of input quantities is small and they are not Gaussian, the PDF of y can be evaluated observing that (3) is the sum of N random variables weighted by their sensitivity coefficients $c_i = \partial f / \partial x_i$; in this case, it is possible to determine the PDF of y by means of the convolution of the PDFs of the input random variables. Naming $g_{X_i}(x_i)$ the PDFs of the random variable X_i, the PDF $g_Y(y)$ of y is

$$g_Y(y) = c_1\, g_{X_1}(x_1) * c_2\, g_{X_2}(x_2) * ... * c_N\, g_{X_N}(x_N). \tag{4}$$

This is the approach used in the numerical experiments.

The sensitivity coefficients can be evaluated by perturbing each input uncertain quantity; this means that in the simulation of a model having N uncertain input quantities, we need to

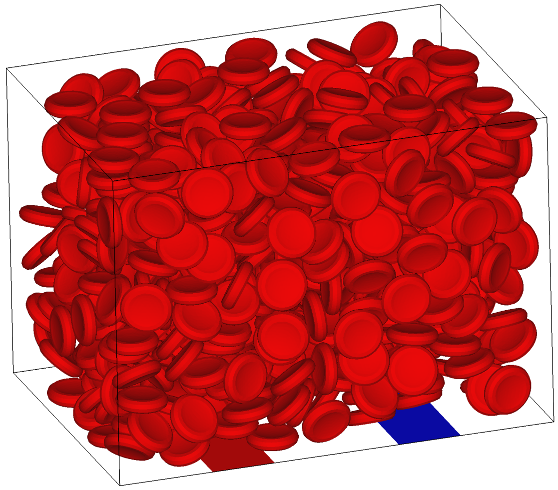

Fig. 1. A portion of a microfluidic channel whose dimensions are $50\mu\text{m}\times 50\mu\text{m}\times 70\mu\text{m}$. In the channel red blood cells flow at a low shear rate. On the bottom of the channel, two gold electrodes $10\mu\text{m}$ wide are used for impedance measurements.

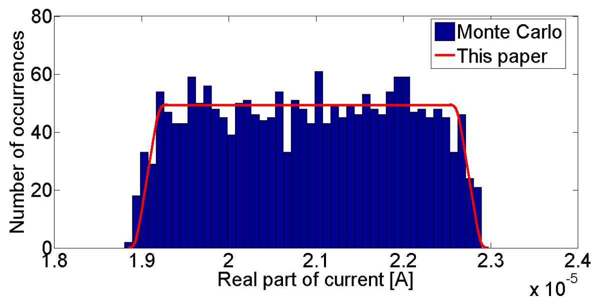

Fig. 2. PDF of the real part of the current.

perform $N+1$ simulations to obtain the PDF of the output quantity.

II. Numerical experiments

As an example, we consider a blood sample flowing with at a low shear rate in a microfluidic channel, see Fig. 1. We compute the uncertainty quantification of the current between the two gold electrodes placed in the bottom of the channel when a known electro-motive force of $1V$ is enforced between them. It is assumed that plasma has a conductivity uniformly distributed in $[0.9, 1.1]$ S/m, the red blood cell (RBC) lipidic membrane uniformly distributed in $[10^{-7}, 10^{-5}]$ S/m and the cytoplasm contained in the RBCs uniformly distributed in $[0.5, 0.7]$ S/m. Concerning the relative electrical permittivities, they are assumed uniformly distributed in $[72, 88]$, $[8.1, 9.9]$ and $[72, 88]$ in the plasma, membrane and cytoplasm, respectively.

A geometric formulation for EQS that includes a surface model for the cell membranes, see [8], is used for the simulations. The domain is discretized with $979,640$ nodes and $5,903,234$ tetrahedra. After the inclusion of the surface model of cell membranes, the unknowns of the resulting complex and symmetric system are $1,582,788$.

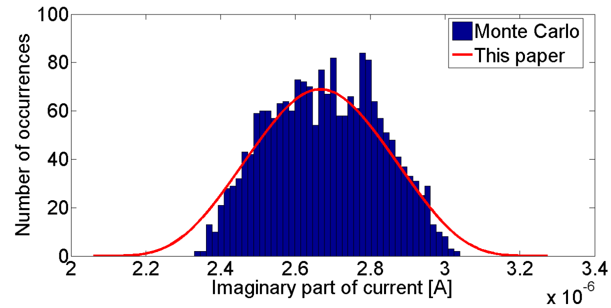

Fig. 3. PDF of the imaginary part of the current.

Each problem is solved in about 128 seconds of wall time including mesh loading, assembling of the sparse matrix, solving the linear system and post-processing for field computation. The time required to perform 2000 simulations with the Monte Carlo method is of roughly 3 days. The proposed method requires 7 simulations for a total time of about 15 minutes.

Fig. 2 shows the behavior of the real part of the current flowing between the electrodes. The histogram shows the number of occurrences over 2000 Monte Carlo simulations and the continuous line is the result obtained using the proposed method. As it can be seen the PDF is trapezoidal since the real part of the current distribution turns out to be dominated by the uncertainties on plasma and cytoplasm conductivities. The membrane conductivity has negligible effects on impedance behavior, but, since the proposed method is very fast, also this uncertain parameter has been simulated without a significant computational effort. Fig. 3 shows the behavior of the imaginary part of the current flowing between the electrodes. As it can be seen the PDF turns out to be almost Gaussian since the imaginary part of the current at this frequency is not dominated by none of the conductivities or permittivities, thus resulting closer to the central limit theorem hypotheses.

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