Project:	**nanoCOPS - nanoelectronic COupled Problems Solutions**
Project Number:	**FP7-ICT-2013-11/619166**
Work Package:	**WP2 : Uncertainty Quantification**
Task:	**T2.2 : EM-Device-Circuit co-simulation with random parameters**
Deliverable:	**D2.4 : Intermediate Report on Methods and algorithms for co-simulation of coupled problems including random parameters without Polynomial Chaos or reduced-order models**
Scheduled:	**M12 (November 2014, Version 1, Submitted 141111)**

Title:	**D2.4 : Intermediate Report on Methods and algorithms for co-simulation of coupled problems including random parameters without Polynomial Chaos or reduced-order models**
	Summary: The report gives an overview of analyzed methods and algorithms for co-simulation of coupled problems including random parameters. The planned applications in nanoCOPS are also shown.
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Date:	**November 11, 2014 (Version 1) February 19, 2015 (Version 2)**

Intermediate Report on Methods and algorithms for co-simulation of coupled problems including random parameters without Polynomial Chaos or reduced-order models

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Version 1: November 11, 2014
Version 2: February 19, 2015

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1 Introduction

The modeling and simulation of coupled multiphysics problems, very often with multiple scales and domains is a key tool, needed in the numerous fields of science and in engineering, for example, see [3, 1, 30, 9, 33]. Multiphysics models can be either described by a single equation with a tightly coupling all the physical phenomena, or, contrary, by a weak form of the coupling system of equations. The multiscale aspect of coupled problems is related to the representation of the various types of physical behavior by means of the different descriptors at different scales. And, finally, in multidomain models, a shared interface is used for the coupling of physical behavior in various regions of space [4].
In today's applications, encountered in electrical engineering, the modeling and simulation of coupled systems is necessary because of the progressive miniaturization and the increasing complexity of components in electronic systems. In this case, depending on the complexity of the analysis, coupled mathematical models of compound devices can be often described by differential-algebraic equations (DAEs), see [2, 11] and partial differential equations (PDEs), see [38, 39]. The common practice, especially popular within the industrial simulators is the application of the so-called companion models [27]. However, this approach gives only a partial insight into field effects. Another solution relies on the direct simulation by the PDE model using the drift-difussion equations for semiconductor devices and the type of Maxwell's equation in the case of distributed devices. Such an approach is required if the operation conditions and the problem scale simultaneously trigger the various physical mechanisms in such a way that a decoupled view introduces to much deviation from reality. For example, the investigation of the thermal-electric coupling or analysis of electric-thermal-mechanic coupling in compound devices was conducted by [6, 16, 28], where, besides typical electric variables such as voltages and currents, the purely non-electric quantities including temperature, stress, strain and dislocations are taken into account. However, by definition, mathematical models are prone to modeling errors. This kind of errors can be treated as uncertainty in models under consideration. The way how the particular part, such as, for example, a core made of nonlinear material of transformer is treated, influences as well very much simulation [22]. Another aspect of uncertainty is a consequence of the measurement process of some electrical quantities that are needed to calibrate models by taking the directly from measurement estimated parameters into account. The latter allows us to describe unknown a priori distributions of modeling parameters, etc. [17]. Finally, the last and probably the most important source of uncertainty results from some imperfections in manufacturing processes including, for example, sub-wavelength lithography, lens aberration, and chemical-mechanical polishing [24]. Thus, the uncertainty quantification (UQ) plays a crucial and key requirement in realistic and predictive simulation of coupled problems encountered in electronic devices.

1.1 Coupled multiphysical problems in nanoelectronics

The coupling of various physical phenomena in nanoelectronics plays an important role in the reliability assessment including the circuit and systems level [37, 15]. Specifically, this is the case for high-performance applications such as CPUs and RF-circuits but also for applications in hostile environment related to automotive industry. In both

cases various types of coupled effects exist. For instance, electro-thermal coupling is of a great importance in operational cycles. Here, on the one hand, a generated substantial amount of heat affects the voltage and current distribution. On the other hand, it also has an impact on the sources of the heat itself. The electro-thermal-stress coupling is investigated in the modeling of a power-MOS device both in DC and in the transient regime, while taking the environmental aspects such as metal stack and package into account.
Consequently, designs in nanoelectronics often lead to large-size simulation problems and include strong feedback couplings. In this case, the modeling methodology for such coupled problems starts with refined modeling, which results in so-called Partial-Differential-Algebraic Equations (PDAEs). To solve these coupled PDAE models numerically, various methods have been proposed. Often a monolithic approach, i.e., the solution of all subproblems at once, might be complicated or even unfeasible due to incompatibility of applied algorithms or software packages. From this viewpoint, such simulations need to be portioned into coupled subproblems in an efficient and stable way, where subdomains are solved separately. In the consequence, this results in a splitting error, which needs to be mitigated by an iterative procedure. The most well-known examples are splitting schemes for linear systems of equations such as Gauss-Seidel or classical domain decomposition methods. In more complex scenarios the decoupling may be relaxed to allow also for independent transient behavior, which leads to dynamic iteration schemes [37]. The complexity of the problems related to the modeling methodology, based on the various mathematical approaches, is schematically shown on Fig. 1. Industry demands the provisions of variability to guarantee quality and yield. It also requires the incorporation of higher abstraction levels to allow for system simulation in order to shorten the design cycles, while at the same time preserving accuracy.

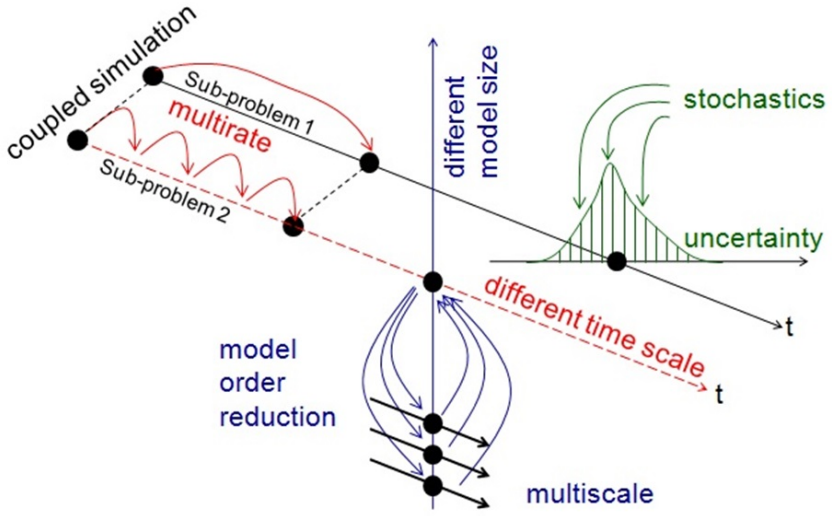


Figure 1: Schematic of a coupled problem (consisting of two sub-problems), including uncertainties. In nanoCOPS, those problems are efficiently solved in time domain and probability space with exploitation of their multirate (different time steps) and multiscale behavior (different discretizations). The discretized models lead to different reduced models by techniques from Model Order Reduction (MOR). Parameterized MOR guarantees the ability to properly deal with the uncertainties in parameters, geometries, and coupling quantities [20].

Fig. 2 shows, for example, a Python-C++ interface, developed by the Humboldt Universität zu Berlin and MAGWEL, for a coupled EM-circuit simulation. It allows for a monolithic transient simulation of lumped circuit equations (resulting from the Modified Nodal Analysis [27]), coupled with the electromagnetic field equations (using vector potential formulation). The simulation has as bottleneck a huge dimensional, non-symmetric Jacobian matrix, where standard direct and iterative linear solvers fail. However, one can exploit a certain Jacobian block structure that allows for a hybrid linear solving combining direct and iterative methods [20, 46].

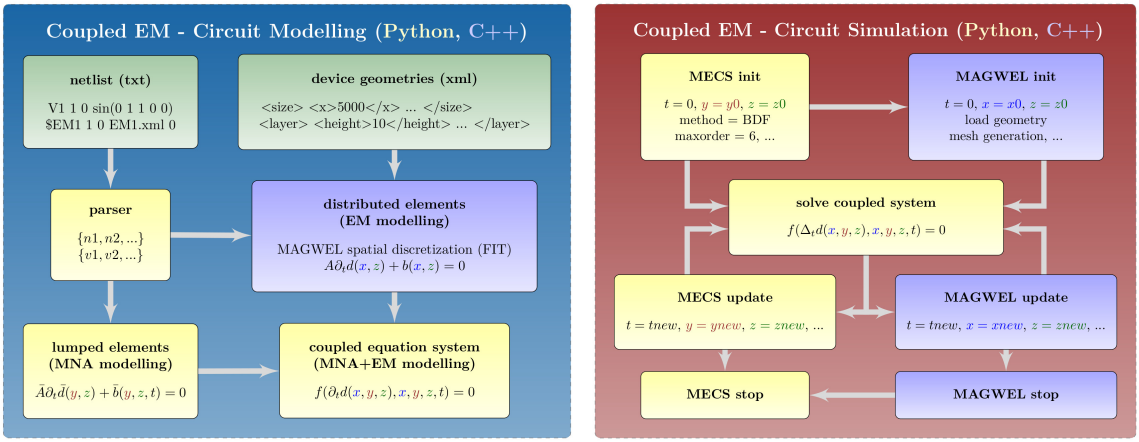


Figure 2: Overview modeling (left) and flow implementation (right) for monolithic coupled simulation [20, 46].

1.2 Stochastic coupled problems description

Let us consider a time-dependent coupled problem, in general described by two operators $\mathbf{F}_1$ and $\mathbf{F}_2$, which can represent the ordinary differential equations (ODEs), the differential algebraic equations (DAEs) or the partial differential equations (PDEs) after a semidiscretizations in space, in the form

$$\mathbf{F}_1(\mathbf{y}_1(t,\mathbf{p}), t, \mathbf{p}) = \mathbf{0}, \tag{1a}$$
$$\mathbf{F}_2(\mathbf{y}_2(t,\mathbf{p}), t, \mathbf{p}) = \mathbf{0}, \tag{1b}$$

where some parameters $\mathbf{p} \in \Pi \subseteq \mathbb{R}^Q$ are involved. The time derivatives are included in each part of systems (1). Furthermore, we assume that each of the operators $\mathbf{F}_i$, for $i = 1, 2$, consists of n_i equations with given initial values for all $\mathbf{p} \in \Pi$. Then, the solution of the system (1) is expressed by $\mathbf{y}_i : [t_0, t_{\text{end}}] \times \Pi \to \mathbb{R}^{n_i}$ with **the coupling variables being a subset of** $\mathbf{y}_i$, for each $i = 1, 2$. Now, we assume, that some parameters exhibit a certain level of uncertainty in the model described by (1). Therefore, for the uncertainty quantification, these parameters aren replaced by independent random variables

$$\mathbf{p} : \Omega \to \Pi, \quad \mathbf{p}(\omega) = (p_1(\omega), \ldots, p_Q(\omega)) \tag{2}$$

on some probability space $(\Omega, \mathcal{A}, P)$ with a joint density $\rho : \Pi \to \mathbb{R}$. That is, we have Q stochastic parameters with independent probability distributions such as Gaussian, uniform, or beta. Then, the solution of (1) becomes a time-dependent random process

and the statistical information like the expected value and the variance for a function $f : \Pi \to \mathbb{R}$ can be obtained by

$$\langle f(\mathbf{p}) \rangle := \mathbb{E}\left[f(\mathbf{p})\right] = \int_{\Pi} f(\mathbf{p})\rho(\mathbf{p})\, \mathrm{d}\mathbf{p}, \tag{3}$$

and

$$\mathrm{Var}\left(f(\mathbf{p})\right) := \mathbb{E}\left[\left(f(\mathbf{p})\right)^2\right] - \left(\mathbb{E}\left[f(\mathbf{p})\right]\right)^2, \tag{4}$$

provided that the integral (3) over the parameter space is finite. Also integral $\mathbb{E}\left[\left(f(\mathbf{p})\right)^2\right]$ in (4) has to be finite. Consequently, for two functions $f, g : \Pi \to \mathbb{R}$ the expectation operator yields an inner product $\langle f, g \rangle := \mathbb{E}\left(f(\mathbf{p})g(\mathbf{p})\right)$ on $L^2(\Omega)$, see, e.g., [31, 47]. Numerical approximations of (3) and (4) are very often required in a practical computation.

1.3 Non-intrusive uncertainty quantification

Non-intrusive methods belong to the sampling techniques, which require repetitive run of the deterministic solver in order to perform the uncertainty quantification. In each method, however, one of the aims is to compute an approximation of the statistical moments like the mean and the standard deviation, for example, or, alternatively, to find a finite set of coefficient functions, when a polynomial chaos expansion has been used [47].

1.3.1 Monte Carlo method

One of the most popular methods for uncertainty quantification is the Monte Carlo (MC) simulation [13, 25]. The principles of MC methods are based on the Strong Law of Large Numbers and rely on repeated random sampling to obtain numerical results. Given realizations $(\boldsymbol{\xi}_1, \ldots, \boldsymbol{\xi}_K)$ of a sample $(\mathbf{p}_1, \ldots, \mathbf{p}_K)$ of the random variable $\mathbf{p}$, the mean value is estimated by

$$m_K := \frac{1}{K} \sum_{k=1}^{K} f(\boldsymbol{\xi}_k). \tag{5}$$

According to the Strong Law of Large Numbers, one can obtain $m_K \to \mathbb{E}(f(\mathbf{p}))$ for $K \to \infty$, thus the expectation value is approximated by the sample mean $m_K \approx \mathbb{E}(f(\mathbf{p}))$ for sufficiently large K. In this context, the MC or quasi MC techniques [26] are a special case of sampling methods, where the weights are $\omega_k = \frac{1}{K}$ for all k. It is well-known fact that the convergence rate of the MC method is proportional to $1/\sqrt{K}$, where K denotes the number of sampling points. In our computations, this method has been only applied for the validation purposes.

1.3.2 Quadrature-based stochastic collocation

Another approach, which relies also on repetitive run of the deterministic model, is the quadrature-based stochastic collocation method (SCM) [8, 47, 48]. These numerical techniques can be directly derived from the formula (3), when using appropriate

quadrature rules for the integral approximation

$$\mathbb{E}\left[f(\mathbf{p})\right] = \int_{\Pi} f(\mathbf{p})\rho(\mathbf{p})\,\mathrm{d}\mathbf{p} \approx \sum_{k=1}^{K} f(\boldsymbol{\xi}_k)\omega_k =: \hat{\mathbb{E}}\left[f(\mathbf{p})\right], \tag{6}$$

where the quadrature grid points $\{\boldsymbol{\xi}_k\}_{k=1}^{K}$ and the weights $\{\omega_k\}_{k=1}^{K}$ correspond to the probability density function ρ. The effectiveness of the quadrature-based stochastic collocation method is strongly affected by the choice of the quadrature grid points. In a similar way, the higher moments such as the variance can be approximated by

$$\mathrm{Var}\left(f(\mathbf{p})\right) \approx \sum_{k=1}^{K} \left(f(\boldsymbol{\xi}_k)\right)^2 \omega_k - \left(\hat{\mathbb{E}}\left[f(\mathbf{p})\right]\right)^2. \tag{7}$$

Both sampling methods (5) and (6) require only the repetitive run of the existing deterministic solver. However, they differ themselves in the choice of the quadrature grid points and the weights, which has an impact on their efficiency. In our computations, the Stroud-3 formula [43] and the so-called sparse grid method [42], which suffer less from the curse of the dimensionality [47], have been used to approximate (3) and (4).

1.4 Algorithm for the UQ with a black-box model

The flowchart of the implemented quadrature-based stochastic collocation algorithm for the UQ propagation using MAGWEL software as black-box is shown on Fig. 3. It consists of two main part such as the UQ engine[1] and the MAGWEL solver. In the prototyping Python-C++ interface, the communication between them is established by using files. The UQ engine comprises three main sub-routines. In the first of them, so-called UQ settings, the input parameters such as the random parameter described by the mean and the standard deviation should be specified. Next, based on this information, in the UQ Preparation/Simulation main routines, first the quadrature points and the weights are generated. Then, after evaluation of the model parameters at these points, the solution of the deterministic problem using the MAGWEL solver is computed at each quadrature grid point. In the post-processing stage, the statistical moments like the mean value and the variance are calculated using (6) and (7). Additionally, graphs of the probability density function and cumulative density function of the quantity of interest can be generated.
The efficiency of this algorithm can be improved by using a parallel technique, where the task related to deterministic calculation at grid points can be just sent to different cores or processors [10]. Another approach relies on utilizing the previous knowledge on the already computed solutions obtained for collocation points in order to efficiently approximate the remaining solutions by exploiting the smoothness of the solution with respect to the parameters [14, 21].

[1] The first experiments did exploit the UQ Toolkit, `http://www.sandia.gov/UQToolkit/`. Currently we also consider Dakota, `http://dakota.sandia.gov/`. Both, UQ Toolkit and Dakota, are developed at Sandia National Laboratories.

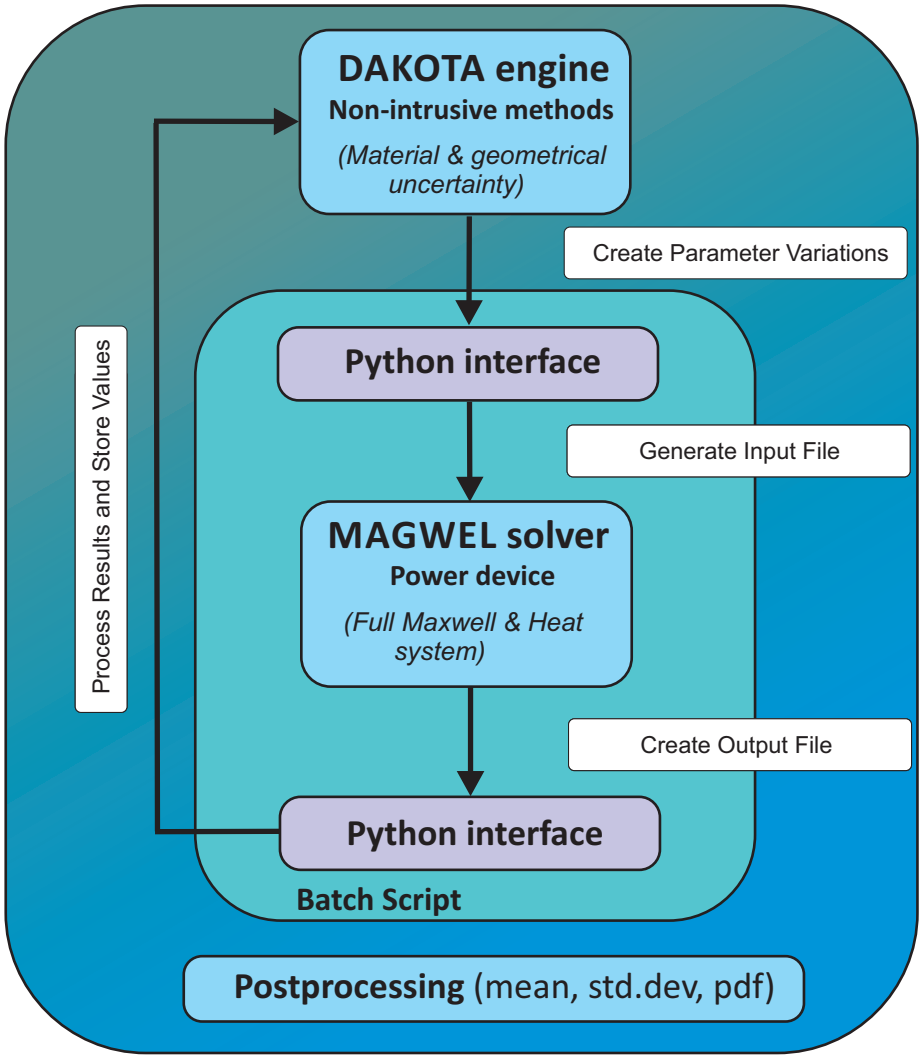


Figure 3: Algorithm for the Stochastic Collocation Method with the MAGWEL solver used as a 'black-box' simulation engine. In the flow indicated above we exploit Dakota, developed at Sandia National Laboratories, `http://dakota.sandia.gov/`.

2 Mathematical Modeling of Stochastic Coupled Systems

In this section, the algorithm for co-simulation of coupled problems including random parameters will be discussed based on three examples: a thermal-circuit coupled problem in Section 2.1, a field-circuit coupling in Section 2.2 and finally an EM-thermal coupled problem in Section 2.3.

2.1 Test Case 1: Transient simulation of a nonlinear thermal-electric circuit with random parameters (UGW/TUD/BUW)

A coupled problem has been investigated, where thermal effects are considered in an electric circuit. Both, the thermal modeling and the particular example, were introduced in [6]. On the one hand, the electric circuit is described by a system of DAEs, as usual. On the other hand, the production as well as conduction of heat is modeled by zero-dimensional lumped elements and one-dimensional distributed elements. The involved one-dimensional heat equation reads as

$$M'(x)\partial_t T = \frac{\partial}{\partial x}\left(\Lambda(x)\frac{\partial}{\partial x}\right) + \text{sources}, \tag{8}$$

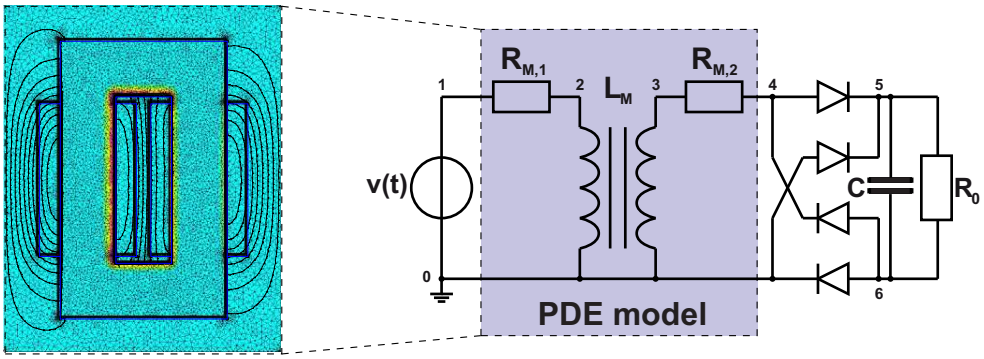
with the temperature T, the thermal conductivity Λ and the thermal mass M'. The properties of the circuit elements depend on the temperature. They also generate energy loss by producing a power contribution in the source terms in (8). It follows a coupled system of DAEs and PDEs. A stochastic formulation was derived, where two random parameters have been introduced: a uniform thermal conductivity in the PDE part (8) and an electric resistance in the DAE part of the circuit equations. Note that the DAE part as well as the coupling conditions are nonlinear, whereas the PDE part is linear. Using a method of lines for the PDE part, it follows a time-dependent coupled system of the form (1). An uncertainty quantification can be obtained straightforward by a quadrature formula in the probability space and transient simulation. A more sophisticated approach is described in [32], where two different quadrature grids for the two subparts have been combined in the time integration.

2.2 Test Case 2: Transient simulation of the field/circuit coupled problem with random parameters (BUW/TUD)

To solve the field/circuit coupled problem, shown in Fig. 4, one approach consists of extracting lumped elements or surrogate models from a field model. By inserting these as a netlist one can exploit a SPICE-like circuit simulator. In [5, 38, 39] co-simulation techniques are exploited to simulate the coupled problem. Alternatively, when no multirate potential can be expected, one will consider monolithic coupling, where field and circuit models are solved together [37].
The stochastic eddy-current field problem, defined in a spatial domain $D \in \mathbb{R}^2$ and a time domain $[t_0, t_{\text{end}}]$, is governed by the random quasi-linear equation

$$\sigma\partial_t \mathbf{a} + \nabla \times \Big((\nu(|\nabla \times \mathbf{a}|)\ \kappa(\boldsymbol{x}, \omega))\ \nabla \times \mathbf{a} \Big) = \boldsymbol{\chi}\mathbf{j}, \tag{9}$$

where $\omega \in \Omega$ denotes the random inputs of the model, $\mathbf{a} := \mathbf{a}(\boldsymbol{x}, t, \omega)$ is the magnetic vector potential (with homogeneous Dirichlet conditions), σ and ν are conductivity and



(a) 2D transformer FEMM **(b) rectifier circuit with embeded FEMM model**

Figure 4: Nonlinear Field/Circuit configuration [5, 38] using FEMM [23] as prototype field simulator.

reluctivity, respectively. Additionally, the function $\kappa(\boldsymbol{x}, \omega)$ has been introduced in order to model the local degradation of material. It has been parameterized by a truncated Karhunen-Loève Expansion (KLE) [18, 41] with N terms, i.e.,

$$\kappa(\boldsymbol{x}, \omega) \approx \overline{\kappa}(\boldsymbol{x}) + \sum_{i=1}^{N} \hat{\kappa}_i(\boldsymbol{x}) \boldsymbol{Z}_i(\omega), \tag{10}$$

where $\overline{\kappa}(\boldsymbol{x})$ denotes the mean of the random field, the functions $\hat{\kappa}_i(\boldsymbol{x})$ are determined by the eigenvalues and eigenfunctions of the assumed covariance function, e.g., the exponential covariance function, and $\boldsymbol{Z}_i(\omega)$ are uncorrelated [47]. In eq. (9), the winding functions $\boldsymbol{\chi} = [\boldsymbol{\chi}_1, \ldots, \boldsymbol{\chi}_l, \ldots, \boldsymbol{\chi}_L]^\top$ are functions of space that distribute the lumped currents $\mathbf{j} = [j_1, \ldots, j_l, \ldots, j_L]^T$ in the 2D domain [40]. To establish the circuit coupling we calculate

$$\partial_t \int_D \boldsymbol{\chi}_l \mathbf{a} \, \mathrm{d}x + R_l j_l = v_l \qquad l = 1, \ldots, L, \tag{11}$$

where $R_l j_l$ is some voltage loss. Each conductor has its own conductance and R_l is given by $\int_D \frac{1}{\sigma_l} \boldsymbol{\chi}_l \cdot \boldsymbol{\chi}_l dx$, see eq (17) in [40].
The v_l in (11) are the couplings to the circuit system of stochastic differential-algebraic equations [38, 39]

$$\begin{aligned} \mathbf{A}_\mathsf{C} \mathrm{d}_t \mathbf{q}_\mathsf{C}(\mathbf{A}_\mathsf{C}^\mathrm{T} \mathbf{u}, t) + \mathbf{A}_\mathsf{R} \mathbf{g}_\mathsf{R}(\mathbf{A}_\mathsf{R}^\mathrm{T} \mathbf{u}, t) + \mathbf{A}_\mathsf{L} \mathbf{i}_\mathsf{L} \\ + \mathbf{A}_\mathsf{M} \mathbf{j} + \mathbf{A}_\mathsf{V} \mathbf{i}_\mathsf{V} + \mathbf{A}_\mathsf{I} \mathbf{i}_\mathsf{s}(t) = \mathbf{0}, \\ \mathrm{d}_t \boldsymbol{\Phi}_\mathsf{L}(\mathbf{i}_\mathsf{L}, t) - \mathbf{A}_\mathsf{L}^\mathrm{T} \mathbf{u} = \mathbf{0}, \\ \mathbf{A}_\mathsf{V}^\mathrm{T} \mathbf{u} - \mathbf{v}_\mathsf{s}(t) = \mathbf{0}, \end{aligned}$$

with additional incidence matrices $\mathbf{A}_*$ such that $v_l = \mathbf{A}_l^\mathrm{T} \mathbf{u}$, or $\mathbf{v} = (v_1, ..., v_L)^\mathrm{T} = \mathbf{A}^\mathrm{T} \mathbf{u}$, for suitable $\mathbf{A}_l$ or $\mathbf{A}$) and constitutive laws for (nonlinear) conductances, inductances and capacitances (random functions with subscripts R, L and C, determined by, e.g., the statistical moments), independent sources $\mathbf{i}_\mathsf{s}$ and $\mathbf{v}_\mathsf{s}$, unknowns are the potentials $\mathbf{u} := \mathbf{u}(t, \omega)$ and currents $\mathbf{i}_\mathsf{L} := \mathbf{i}_\mathsf{L}(t, \omega)$ and $\mathbf{i}_\mathsf{V} := \mathbf{i}_\mathsf{V}(t, \omega)$.
Finally, the stochastic field/circuit coupled problem with the parameters $\mathbf{p}$ substituted by the independent random variables $\mathbf{p}\,(\omega)$ can be rewritten in a set of coupled index-1

DAEs of the form

$$\dot{\mathbf{y}}_i(t,\mathbf{p}) = \mathbf{f}_i(\mathbf{y}(t,\mathbf{p}),\mathbf{z}(t,\mathbf{p}),t,\mathbf{p}), \quad \mathbf{y}(t_0,\mathbf{p}) = \mathbf{y}_0(\mathbf{p}), \tag{12a}$$

$$\mathbf{0} = \mathbf{g}_i(\mathbf{y}(t,\mathbf{p}),\mathbf{z}(t,\mathbf{p}),t,\mathbf{p}), \quad \mathbf{z}(t_0,\mathbf{p}) = \mathbf{z}_0(\mathbf{p}) \tag{12b}$$

with the differential variables $\mathbf{y}_i : [t_0, t_{\text{end}}] \times \Pi \to \mathbb{R}^{Ny_i}$ and the algebraic variables $\mathbf{z}_i : [t_0, t_{\text{end}}] \times \Pi \to \mathbb{R}^{Nz_i}$ for $i = 1, 2$. Consequently, the solution of this initial value problem, $\mathbf{x}(t,\mathbf{p}) := (\mathbf{y}(t,\mathbf{p}),\mathbf{z}(t,\mathbf{p}))^\top : [t_0, t_{\text{end}}] \to \mathbb{R}^{Ny} \times \mathbb{R}^{Nz}$, depends on time as well as the random parameters.

2.3 Test Case 3: Transient simulation of an electro-thermal coupled problem based of a Power MOS Transistor with random parameters (BUW/MAG)

The implementation at MAGWEL deals with the electro-thermal coupling problem in an ab-initio self-consistent manner [19, 36]. In this case, electrical and thermal equations are solved simultaneously and self-consistently from a single set of equations. Accurate modeling of metal layers as required for advanced integrated BCD (Biploar-CMOS-DMOS) technologies has been obtained by the application of a high spatial resolution. At the same time, the simulator uses a well-adopted mesh for the substrate, which is important for the simulation of the temperature. Consequently, both the voltage drop in the on-chip metallization and the device temperature can be determined without sacrificing accuracy. Joule self-heating and heat flow in metal is modeled together with non-linear temperature-dependent electrical and thermal resistivity and thermal capacitances of materials [7, 19]. The electrical part of the integrated field solver [19, 29] addresses the current-continuity equation and Ohm's law

$$\nabla \cdot \mathbf{J} = 0, \qquad \mathbf{J} = \sigma(T)\mathbf{E}, \tag{13}$$

where $\mathbf{J}$ and $\mathbf{E}$ denote the current density and the electrical field, respectively, and σ is the temperature-dependent electrical conductivity. The thermal part of the solver refers to the heat equation which is controlled by Joule's law

$$\partial_t U = -\nabla \cdot Q + Q_e, \quad Q = -\lambda \nabla T, \quad U = C_v(T - T^*), \tag{14}$$

where the local heat generation is defined by $Q_e = \mathbf{J} \cdot \mathbf{E}$. Furthermore, C_v is the constant-volume heat capacitance of the material, T refers to the reference or ambient temperature, λ represents the thermal conductivity. The Neumann (adiabatic) boundary condition is imposed on the side walls of the simulation domain. The solution of (14), assuming the heat source is known, provides the needed information about the temperature to (13). The source may comprise several contributors such as the boundaries of the domain with heat-injecting or extracting properties or the Joule self-heating component Q_e. To perform the uncertainty quantification, some parameters $\mathbf{p}$ in the model defined by the coupled system (13) and (14) have been substituted by independent random variables $\mathbf{p} = (\epsilon(\omega), W_k(\omega), \sigma_k(\omega), C_v(\omega)))$ defined on some probability space. Consequently, the model for a semiconductor device [45, 35] stated on a bounded domain $D \subset \mathbb{R}^d$ is governed by the coupled stochastic partial differential equations (PDEs)

$$\begin{cases} \nabla \cdot (\epsilon \nabla V) = \rho, \\ \nabla \cdot \mathbf{J}_{(p)} + q\partial_t p + qR(p,n) = 0, \\ \nabla \cdot \mathbf{J}_{(n)} - q\partial_t n - qR(p,n) = 0, \\ \mathbf{J}_{(n,p)} = q\ (n,p)\ \mu_{(n,p)} \cdot \nabla V \pm qD_{(n,p)} \nabla (n,p), \\ C_v \partial_t T = \nabla \cdot \lambda(T) \nabla T + \sigma(T) \|\nabla V\|^2, \end{cases} \tag{15}$$

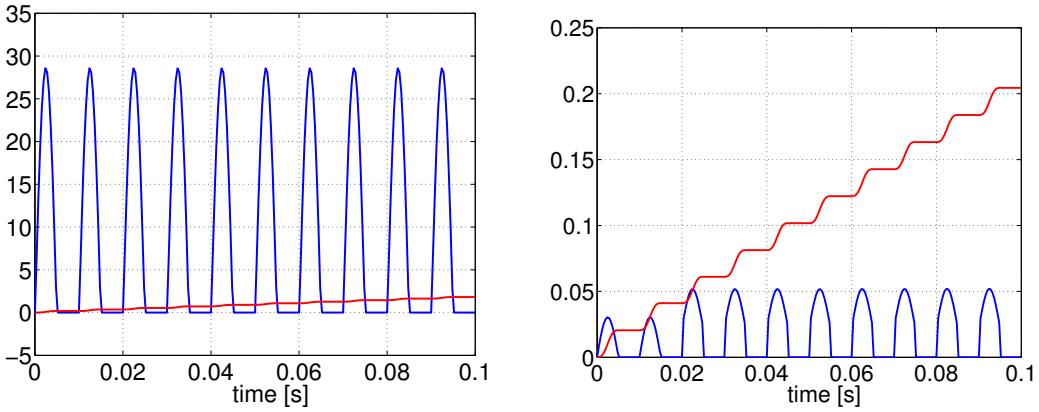


Figure 5: Expected values (left) and standard deviations (right) for the output voltage (blue) and the dissipated energy (red).

equipped with suitable boundary conditions, where ρ, ϵ and q denote the charge density, the permittivity and the elementary charge, respectively. In this model, generation-recombination processes are involved by the recombination rate R, for example, the Shockley-Read-Hall term.The electrical field $\mathbf{E} := \mathbf{E}(\boldsymbol{x}, t, \omega)$ is determined by the electric scalar potential $V := V(\boldsymbol{x}, t, \omega)$. Furthermore, n and p, represent the concentration of holes and electrons, while D_n, D_p, μ_n, μ_p, $\mathbf{J}_n := \mathbf{J}_n(\boldsymbol{x}, t, \omega)$, $\mathbf{J}_p := \mathbf{J}_p(\boldsymbol{x}, t, \omega)$ are the diffusion, mobilities and currents densities of electrons and holes, respectively. The symbol (n, p) describes in compact way equations for electrons and holes. In this case, also temperature is defined as $T = T(\boldsymbol{x}, t, \omega)$. For the k-th conductive layer of the model, the σ is represented by $\sigma = W_k \sigma_k$, where W_k denotes the size of the layer, for example, the thickness.

3 Preliminary results of the UQ propagation in the coupled problems

3.1 Test Case 1: Results of the UQ transient analysis for the thermal-electric circuit problem of Section 2.1

The coupled problem of an electric circuit including thermal effects has been simulated in case of random parameters as described in Section 2.1. The quadrature approach using differerent grids for the subparts yields approximations for the expected values and the standard deviation. Some results at important components of the DAE part and the PDE part are depicted in Fig. 5 and Fig. 6, respectively. The output voltage exhibits an oscillatory behavior, since a sinusoidal input voltage was used. As expected, the dissipated energy increases monotonically in time. The heat production and heat dissipation can be observed in the one-dimensional temperature of the resistor. More details on this transient simulation can be found in [32].

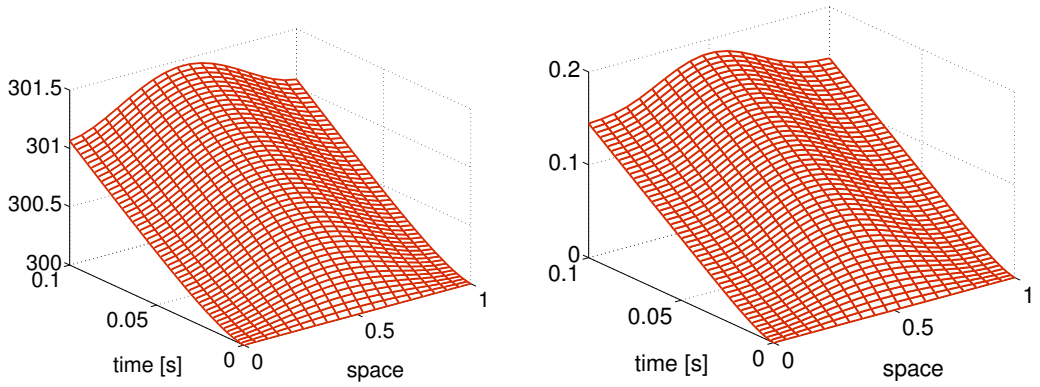


Figure 6: Expected value (left) and standard deviation (right) of temperature in a resistor.

3.2 Test Case 2: Results of the UQ transient analysis for the field/circuit coupled problem of Section 2.2

In the application of the bridge rectifier with the low pass filter, shown in Fig. 4a, the model of the single-phase isolation transformer with the laminated steel core has been used as the field device. Its geometrical and material parameters can be found in [38]. For the purpose of the simulation, the software package FEMM [23] has been applied. The attached diode bridge circuit, depicted on Fig. 4b, has been excited by a sinusoidally varying voltage source $u(t) = 120\sin(\omega t)$ V with $\omega = 2\pi$ kHz. The diode current-voltage characteristic is described by the Shockley diode equation

$$i = I_{\mathsf{S}} \cdot (\exp(v/V_{\mathsf{th}}) - 1) + G \cdot v, \tag{16}$$

with the conductance $G = 10^{-12}$ S, the saturation current $I_{\mathsf{S}} = 10^{-9}$ A and the thermal voltage $V_{\mathsf{th}} = 0.26 \cdot 10^{-3}$ V. In order to reduce the ripple of the output voltage developed across a load resistor $R_0 = 1$ kΩ, a smoothing capacitor $C = 1.3 \cdot 10^{-6}$ F has been connected in parallel with the load resistor. The result of the transient simulation on the time interval from $t_0 = 0$s till $t_{end} = 4.37 \cdot 10^{-3}$s is presented in Fig. 7, while applying a monolithic approach. All time-integration has been computed by the Backward Euler method with a fixed time step size $\Delta t = 2.5 \cdot 10^{-5}$s. To perform the UQ analysis, the nominal parameters of all the four diodes as well as the resistance and the capacitance of the low pass filter have been replaced by

$$\tilde{I}_{\mathsf{S}}(p_1) := I_{\mathsf{S}}(1 + 0.05p_1), \quad \tilde{V}_{\mathsf{th}}(p_2) := V_{\mathsf{th}}(1 + 0.05p_2),$$
$$\tilde{R}(p_2) := R(1 + 0.1p_3), \quad \tilde{C}(p_4) := C(1 + 0.1p_4)$$

with independent, uniformly distributed, random variables $p_j \in [-1, 1]$, for j = 1, ..., 4. Hence, a relatively high uncertainty of 10% or 5% is considered for each parameter. The same procedure has been conducted for other stochastic parameters (with the variance of 10% for each component) related to the first seven components of the KLE that capture 95% of the random field energy. For the purpose of modeling of the transformer core, we consider a random field of reluctivity with one mean and an exponential two-point covariance function

$$C(\mathbf{x}, \mathbf{y}) = \delta^2 \exp(-\|\mathbf{x} - \mathbf{y}\|_2 / L), \tag{17}$$

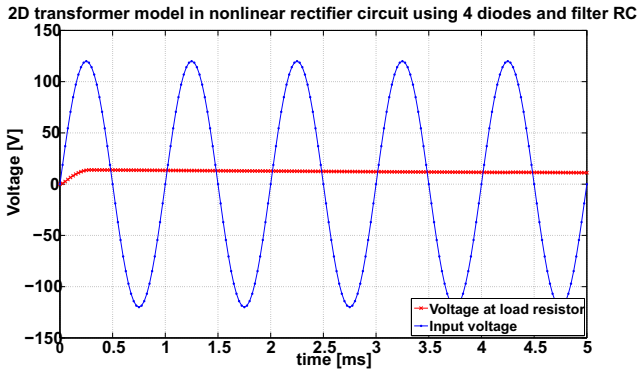


Figure 7: Output/input relation in a bridge rectifier with RC filter.

with δ = 0.1 and L=10 being the correlation length. This resulted in 22 deterministic transient simulations of a rectifier circuit model. In each simulation, the degradation of an iron core of the transformer has been taken into account using a KLE dimension-reduction technique. Fig. 8 presents the approximation of the mean and standard deviation obtained by the numerical simulation using the non-intrusive method (SCM).

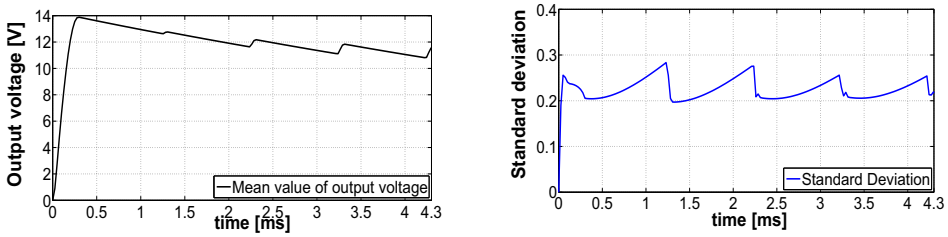


Figure 8: Expected value and standard deviation of the solution of the bridge rectifier with random parameters.

The result of the variance-based sensitivity analysis [44] is depicted on Fig. 9. It shows that the output voltage is more or less equally sensitive to all considered parameters.

3.3 Test Case 3: Results of the UQ transient analysis for the Power Transistor model of Section 2.3

The problem with uncertainty quantification of both material and geometrical parameters comes from the automotive industry, where there is a need to handle the demanding electro-thermal operational constraints to design both components and systems. First, a similar structure to the one proposed in *Use Case I: Power-MOS - electro-thermal-stress coupling*, shown in Fig. 10(b), has been considered as a case study. The geometrical finger structure of a device design has been shown in Fig. 10(a). For uncertainty quantification, the coupled problem defined by stochastic PDEs (15) is solved by the deterministic MAGWEL solver [19] at every quadrature grid point using a type of the stochastic collocation method. In the case of the uncertainty of geometry, the thickness variation has been modeled by Gaussian distribution. The nominal and mean value as well as the standard deviations caused by uncertain geometry have

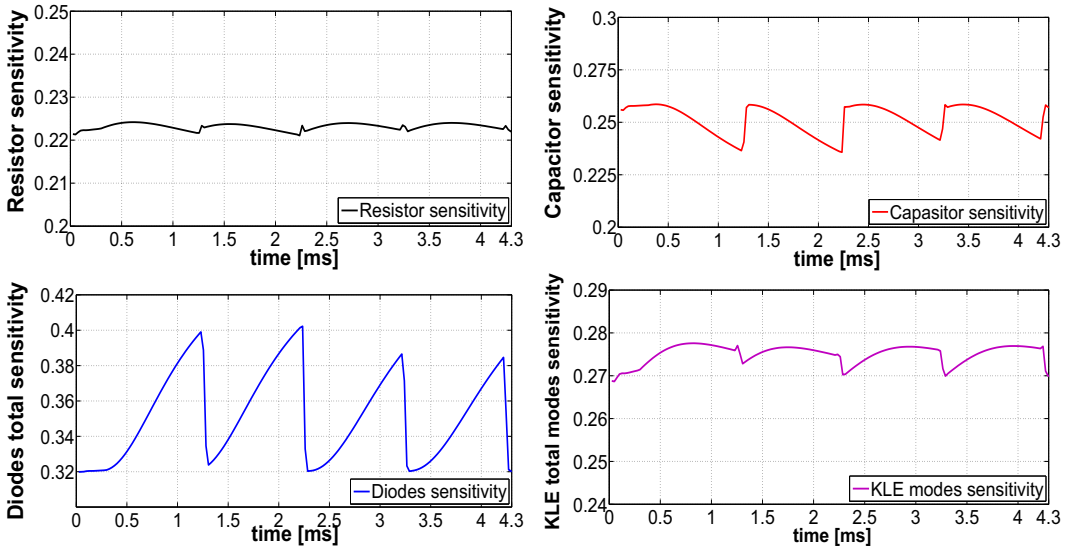


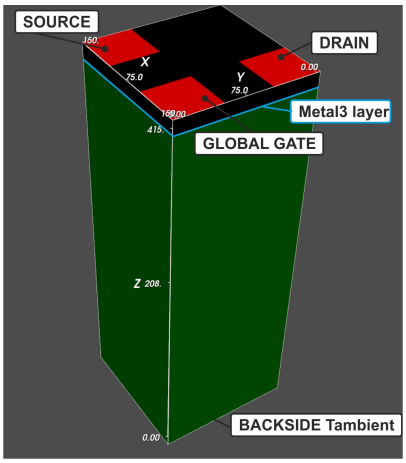
Figure 9: The variance based sensitivities calculated for the resistance, capacitor and diodes parameters and of the KLE components.

been shown on Fig. 11. A similar analysis has been performed when conductivity is treated as uncertain parameter. The UQ propagation in the part of the power device caused by conductivity variation is presented in Fig. 12.

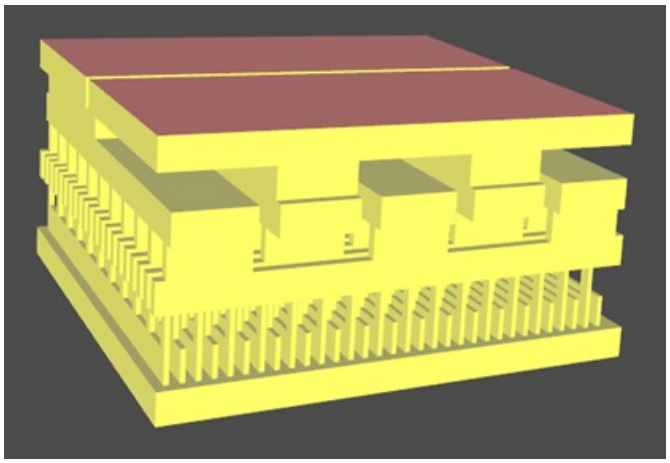
4 Planning

Between M6-M12 implemenation did start. Based on experiences further, refined, choices will have to be made on best methods to be chosen. Also new methods may have to be developed. Especially on including parameterized Model Order Reduction (PMOR) we refer to the deliverables D1.1 and D2.2 [7, 34] and to ideas in [21]. In D2.2 it was noted that geometrical variations may require some restrictive assumptions due the effect on the computational mesh in the general case. Hence next steps will be

- PMOR for (linear) electromagnetics, or heat or circuit parts. First results here look promising.
- PMOR for nonlinear problems. Especially in the heat coupling we can exploit special MOR techniques for quadratic nonlinearities, developed by MPG. These are currently being extended to parameterized versions.
- Geometrical and material variations. We will NOT use topology perserving finite element methods. Such methods are available and are also used within other projects on other types of examples. They are, however, less relevant for the nanoCOPS problems and carrying them over would requires major adaptations to the vendors software packages.



(a) Part of the finger structure in a typical device of a power transistor.



(b) Case I: The geometry of the power transistor.

Figure 10: The layout of the power transistor [19].

5 Risks

First experiments with topology optimization learned us how to technically combine the UQ with FEM/Finite Volume/FIT discretizations. We have also seen that for geometrical variations UQ by the Stochastic Collocation Method can become much less trivial than expected: the method can become intrusive - which, clearly, will become a point of attention by our industrial partner MAGWEL. An intrusive step demands severe code adaptations comparable to developing dedicated interfaces as is done in WP1 for integrating circuit/field simulation tools.

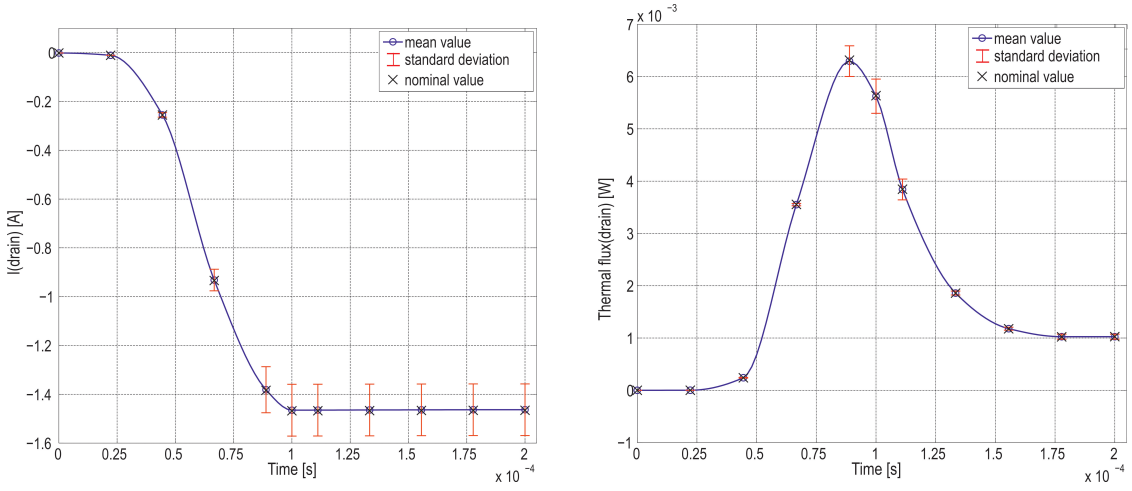


Figure 11: UQ analysis for the thickness of the Metal3 layer modeled by a Gaussian distribution with 10% variation around a nominal value 1μm.

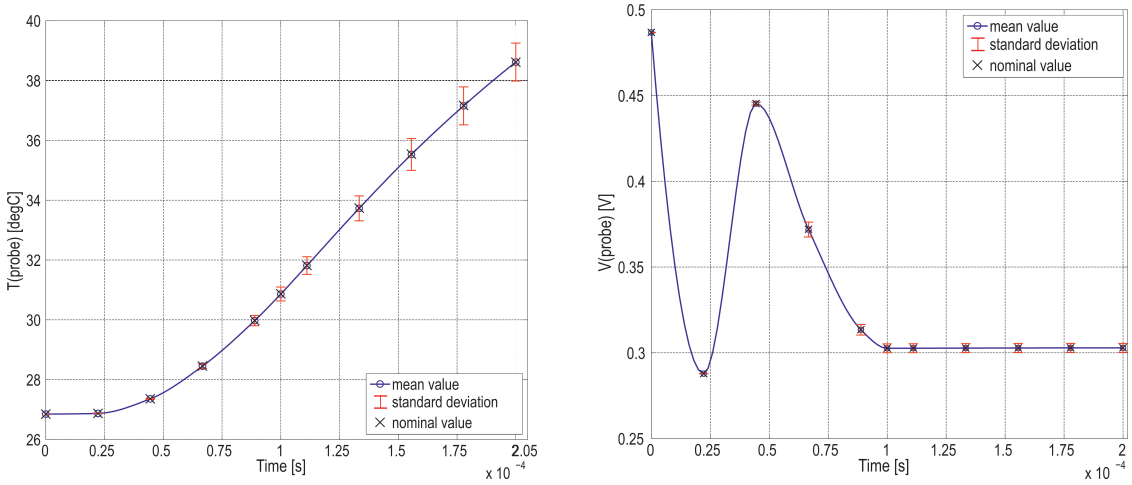


Figure 12: UQ analysis for σ_k (of the Metal3 layer) modeled by a uniform distribution with 15% variation around a nominal value 2e7 S/m.

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