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Design for Reliability and Robustness through Probabilistic Methods in COMSOL Multiphysics with OptiY

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Abstract: One challenge in designing micro-electro-mechanical systems (MEMS) is considering the variability of design parameters caused by manufacturing tolerances and material properties. The function of MEMSs is significantly influenced by this variability, which can be represented in terms of statistical variables. In order to involve statistical design parameters into the design optimization process we use probabilistic approaches. Monte Carlo Sampling, Response Surface, and Moment methods will be described. We applied the methods to a thin-film resonator as an example to show how to analyze the influence of scattering design parameters on the behavior of the resonator. We used a COMSOL Multiphysics model, which computes the first resonance frequency. For performing the probabilistic simulation, the model is coupled to OptiY via a script interface.

Keywords: Robust Design, Reliability Design, Probabilistic Design, Optimization, MEMS.

1. Introduction

The properties within a set of realizations of a technical design scatter randomly. Variability, or uncertainty of the design parameters are caused by manufacturing inaccuracy, process instability, environmental influences, human factors, etc. This aspect is considered in the design process by statistical concepts. Classic simulation and local sensitivity analysis cannot sufficiently predict the real system's behavior caused by the variability of the design parameters. A probabilistic simulation, however, calculates the probability distributions of functional variables from any type of probability distributions of the design parameters (Figure1).

Using a probabilistic approach, the designer no longer thinks of each variable to be a single value. Instead, each variable is assumed to be a probability distribution. From this point of view, probabilistic design predicts the flow of variability through a system. To improve the design quality, the designer has to adjust the design aiming at reducing the flow of random variability. Such an approach enables to predict and rectify many quality problems in early design stages at reduced cost.

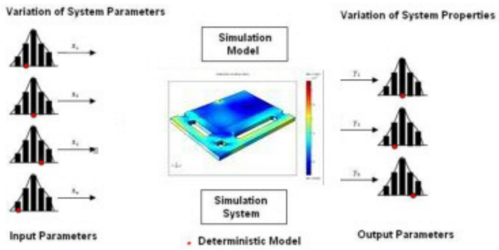

Figure 1. Natural variability of technical systems.

2. Why design for reliability and robustness of MEMS

Today's micro electromechanical systems (MEMS) fulfill a broad range of functions, based on electromechanical, chemical, optical, biological, and thermo-fluidic effects. Examples are sensors in the automotive industry, surgical devices and implantable biosensors in medicine, optical switches and RF waveguides in telecommunications and navigation applications. Major hurdles for commercialization are low reliability, robustness, and quality. In optimizing the design of a MEMS that is robust against scattering of material properties, design dimensions, properties of technology steps, or ambient conditions all that properties have to be considered with their distribution functions. Considering the scattering of the properties is more important in MEMS design, compared to classic technical systems, because of the facts that [3, 5]:

- The scattering of the design and process parameters is relatively large, compared to the dimensions of the system,
- The functionality is highly influenced by the tolerances,
- Many materials are poorly characterized.

Therefore, to ensure maximum product performance, a reliability and robustness design tool is desirable which considers specified distribution functions of the properties.

3. Probabilistic Methods

For deterministic input-output relations, probabilistic methods are used to calculate the distributions of output variables from a given set of stochastic distributions of input variables. We present two classes of probabilistic methods provided by the multidisciplinary analysis and optimization program OptiY [1]: Response-Surface and Moment methods, and we compare them to Monte Carlo sampling. There are also a lot of other reliability methods such as FORM, SORM, mean value etc. [4]. These methods provide only limited information, and will not be dealt with in this paper.

3.1 Monte Carlo sampling

Monte Carlo sampling applies a random number generator to generate the input distributions. There are several types of random number generators: plane Monte-Carlo, Latin-Hypercube and Sobol. The model calculation has to be performed for each input sample, to obtain the output sample. The output distributions have to be statistically calculated from the output sample. This is quite simple to arrange and does not put great demands on the model, not even an input-output-relation is required. Unfortunately, Monte Carlo sampling converges very slowly. Thousands of model calculations are required to obtain accurate output distributions. Results computed by Monte Carlo sampling are stochastic and instable, because they depend on the specific sample set. Therefore, this method is not recommended for robust design optimization.

3.2 Response Surface Methodology

Time-consuming simulations solely provide point-wise information about input-output relations in the design space. To explore the entire design space and reduce the computational burden, global approximation methods are applied. These approximations are also known as metamodel or surrogate model. A metamodel replaces the true functional relationship with the mathematical expression y(x), the so-called response surface, which is much easier to compute. There are different metamodel types: Polynomial, kriging, radial basis function, neural network, etc. They differ in the mathematical expressions that describe the output variable as a function of the input variables. Which metamodel type should be applied depends on the true input-output-relationship. We use here the polynomial metamodel in any order, which is easy to employ and able to represent robust most global input-output-relationships for the response surface methodology. For example, the second order polynomial can be explained:

$$y = \beta_0 y_0 + \sum \beta_{1i} x_i + \sum \beta_{2i} x_i^2 + \sum \beta_{ij} x_i x_j$$

For the generation of the metamodel, that means computing the unknown factors β of the polynomial, an appropriate number of sampling points is needed. These so-called support points can be selected via different design of experiment techniques (DoE) in order to gain maximum information on the characteristics of the underlying relationship. For each point, the time-consuming simulation of the model is performed to get the true value of the response variable y. For the second order polynomial, $\mathbf{n}^2/2+3\mathbf{n}/2+1$ model calculations are required, where **n** is the number of input variables. To fit the metamodel with the unknown factors β to the support points, the least square method or so-called linear regression analysis is used.

The probability distribution of the output variable y can be gained using the Monte-Carlo sampling with a virtual sample set based on the approximated metamodel. The computing time here is negligible compared to a time-consuming model calculation. The results are very accurate using a high virtual sampling size. But they are still stochastic and instable, because they also depend from the specific virtual sample set. Therefore, the method is only conditionally applicable for a robust design optimization considering reliability.

3.3 Moment Method

The principle of the moment method also bases on the metamodel between input and output. The metamodel type here is the first order or second order Taylor series as polynomial ansatz:

$$f = f_0 + \sum_{j=1}^{n} \frac{\partial f}{\partial x_j}(x_j - x_0) + \frac{1}{2}\sum_{j=1}^{n} \frac{\partial^2 f}{\partial x_j^2}(x_j - x_0)^2$$

To obtain the unknown factors of the Taylor series, the partial derivatives are computed based on the time-consuming model calculations. For each design point, these support points are deterministically fixed. If **n** is the number of input variables, the required number of model calculations for the second order moment method is $2\mathbf{n}^2+1$. Instead of Monte-Carlo sampling, the k-th center moments of the output will here be numerically calculated based on the approximated Taylor series for the output distributions:

$$\mu_k = \int_{\infty}^{\infty} (x - x_0)^k f(x)dx$$

The output distributions can be fitted using the well-known table of the moments. State of the art is that an arbitrary probability distribution can only be fitted using four center moments. Therefore, only second order Taylor series can be used for the moment method achieving accurate fitting of a distribution. This is a limitation of the moment method compared to response surface methodology. But the moment method is adequate for most cases of simulation. The computing time of this method is also very fast. The results are analytically calculated and therefore very accurate and definitely stable. This method allows fast robust design optimization [2].

4. COMSOL Multiphysics model of a Thin Film Resonator

The thin film resonator consists of a shuttle and four straight cantilevers fixed on the outer sides. Almost all surface-micro-machined thin films are subject to residual stress. The most common is thermal stress, which is caused by a difference in the coefficients of thermal expansion of the film and the substrate. Here we study the first resonant frequency of the resonator depending on the residual stress with a 3D COMSOL Multiphysics structural mechanics model.

In order to solve the eigenfrequencies with the residual stress, the large-deformation analysis is used. In the first step, the residual stress is computed by a linear solver and stored. The second step calculates the eigenfrequencies involving the stored linear solution. The simulation uses the nominal values of the design parameters given in Table 1. The result is a first resonant frequency of about f1=19 kHz (Figure 2).

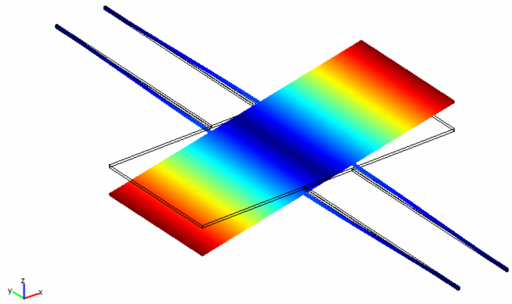

Figure 2. First resonant frequency at 19 kHz

5. Probabilistic Simulation

We consider now the natural variability and uncertainty of the resonator via probabilistic simulation coupling with OptiY [1]. It is assumed that the material properties and environment influences are uniformly distributed and all manufacturing tolerances are normally distributed (Table 1). The goal is to explore the design at the nominal point within the tolerance space due to variability and uncertainty. The failure mechanisms of MEMS depend on individual components and should therefore be defined individually. For the thin film resonator, the reliability and robustness is characterized by the first resonant frequency f1 ≥ 18 kHz.

Design Parameter	Nominal Value	Tolerance Value	Stochastic Distribution
Young's modulus **E** (GPa)	155	15.5	Uniform
Density **rho** (kg/m^3)	2330	200	Uniform
Residual stress **sigma** (MPa)	50	5	Uniform
Deposition Temperature **T1** (K)	678.15	200	Uniform
Shuttle Length **Ls** (µm)	250	0.5	Normal
Shuttle Width **Ws** (µm)	120	0.5	Normal
Cantilevers Length **Lc**	200	0.5	Normal

(µm)			
Cantilevers Width **Wc** (µm)	2	0.5	Normal

Table 1. Design parameters of the resonator

5.1 Coupling COMSOL-OptiY

To couple COMSOL Multiphysics with OptiY, the resonator model must be saved as script file (resonator.m). Then define the parameters in the script file und replace all adequate model data by these parameters. For examples:

E = 1.55E+11;

rho = 2330;

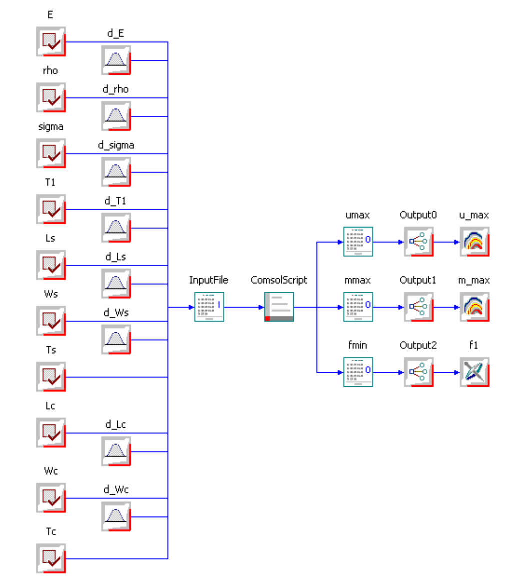

Figure 3. Process workflow

To accerelate the simulation, all commands for post-processing are deleted from the script file. Then at the end of the script file insert a command to save the first resonant frequency to another ASCII-file (fmin.txt):

fmin = postmin(fem,'eigfreq_smsld');

save fmin.txt fmin -ascii -double;

After creating the script file, we build a process workflow in OptiY (Figure 3). The script file (resonator.m) is linked as Input-File and the ASCII-file (fmin.txt) as Output-File. The Extern-Script in OptiY is to start COMSOL-simulation containing following codes:

comsol batch resonator

With this command, COMSOL will start in batch mode and execute the script file (resonator.m) completely.

5.2 Simulation Results

Probabilistic simulation is performed using several model calculation loops in COMSOL. The number depends on the used probabilistic method. For the resonator, the first order polynomial ansatz without input-interaction is used due to the linear correlation between inputs and output. Only 9 model calculations are needed for 8 stochastic variables. The computing time is acceptable also for large models.

Firstly, we compare the cumulative distribution functions (CDF) of the resonant frequency obtained from response surface methodology and the moment method. Both methods yield the same results (Figure 4). That points to correctness and high accuracy of all numerical methods implemented in OptiY.

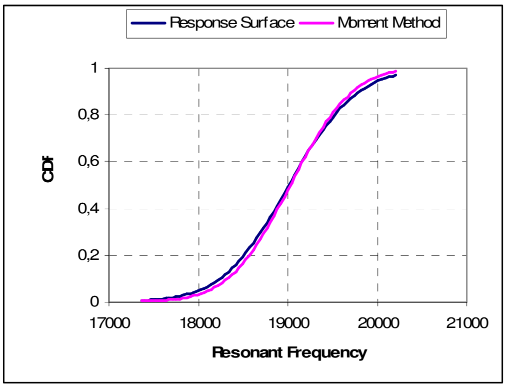

Figure 4. CDF of the resonant frequency by response surface and moment method

We get here a normal probability distribution function (CDF) of the first resonant frequency f1. Its mean value calculated by COMSOL Multiphysics is 19 kHz. But the probabilistic analysis furnishes a variation from 17 kHz to 20 kHz in the reality (Figure 5). Although the deterministic simulation shows the satisfaction of design requirements, its variability may violate the defined boundary ($f1 \geq 18$ kHz). In our case, 3% of the resonator at a mass manufacturing process might fail during usage.

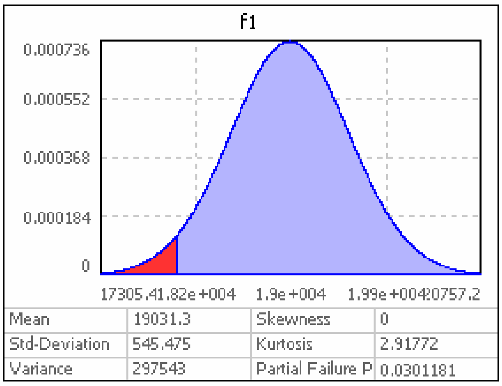

Figure 5. PDF of the resonant frequency

Now, the following question is arising from this result: Which model parameters contribute most to the first resonant frequency variability and, possibly, require additional research to strengthen the knowledge base, thereby reducing output uncertainty. This information is also available. The sensitivity chart shows the parameters of influence on the first resonant frequency in descending order (Figure 6). The variability of the width of the cantilevers, the residual stress, and the material density are significant. Other parameters do not play an important part and can be deleted from the final model.

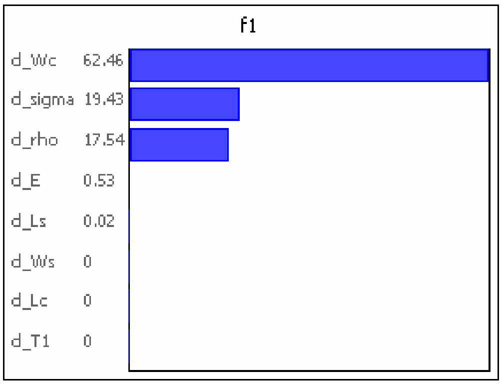

Figure 6. Sensitivity of the resonant frequency

6. Conclusions

We showed shortcomings of today's deterministic simulation. Coupling of COMSOL Multiphysics with OptiY enables the virtual components of MEMS be modeled and simulated closer to reality, using probabilistic methods. The aspects of reliability and robustness can be investigated in early design stages so that cost and time are saved. This is demonstrated with help of a thin film resonator as design example.

7. References

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