Design and Analysis of Computer Experiments for Bulk Acoustic Wave filters: Comparison of several types of Designs and Comparison of Kriging versus Pseudo-cubic Thin-plate type Spline

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Bulk Acoustic Wave (BAW) filters have appeared at the beginning of the 1980's as a result of trials for increasing the frequency of quartz resonators[1,2]. Their principle is to exploit the mechanical resonance of the vibration of a piezoelectric layer for building band-pass filters. The BAW we are interested in may be modeled as a ten layer device. Given the thickness of those ten coats, a numerical simulator computes the response of the filter and gives five responses characterizing the behavior of each filter: Centre Frequency, Bandwidth, Insertion Losses, Ripple and Adaptation (these five responses will be detailed in the full length paper).

Since production hazards usually lead to a difference between the theoretical thickness of the layers and the dimension observed after production, a percentage of the production does not comply with standards and has to be disposed of. The aim of the study is to compute the efficiency of the BAW's production. Even though the statistical distribution of the thickness for the 10 coats is known, a classical Monte Carlo method is unaffordable due to the CPU time of the acoustic and electric simulator. In order to overcome this problem one possibility is to built for each response one metamodel based on a limited number of evaluations (1000) of the simulator. But this leads to new issues: what would be a good Design of Experiment (DOE) for this problem? What kind of metamodel should be used?

We test three types of Design of Experiments (DOE) on this ten dimension example: a DOE based on the combination of composite designs, a space filling design based of MaxiMin Latin Hypercube Sampling (LHS), and another space-filling design, a Halton's low discrepancy sequence. Each of these three DOE has the same number of 1003 points distributed inside a unit hypercube. To get locally accurate metamodels in the center of the domain (which is the region of interest) for the two space filling designs we use a continuous transformation toward the $[-4 ; +4]^{10}$ region of $\mathbb{R}^{10}$ that leads to a higher point density in this region. More details on these three DOE will be given in the full length paper.

We use three types of metamodels: Ordinary Kriging (OK) with gaussian covariance function, Universal Kriging (UK) with gaussian covariance function and Pseudo-cubic Thin-plate type interpolating multidimensional Splines. OK and UK are classical and well known[3] and details of their use are in the full length paper. The Pseudo-cubic Thin-plate type multidimensional Spline is a family of splines proposed by Duchon[4], and consist of a trade-off between smoothing and interpolating splines. In our case, we used the interpolating version of these splines. Experts usually consider that splines are based on energetic considerations and kriging is more based on statistic considerations, but

[1] T.W. Grudkowski, J.F. Black and T.M. Reeder, *Fundamental mode VHF/UHF bulk acoustic wave resonators and filters on silicon*, in 1980 IEEE Ultrasonics Symposium Proceedings, pp. 829-833.
[2] K.M. Lakin and J.S. Wang, *UHF composite bulk wave resonators*, in 1980 IEEE Ultrasonics Symposium Proceedings, pp. 834-837.
[3] T. J. Santner, B. J. Williams, W. I. Notz, *The Design and Analysis of Computer Experiments,* Springer, 2003
[4] J. Duchon, "*Splines minimizing rotation-invariant semi-norms in Sobolev space*", Lecture Notes in Mathematics, vol 571, pp85-100, 1977

it must be noticed that the two overall mathematical objects are not so different. Both are mainly based on radial basis functions.

With this type of spline, there is no constraint on the repartition of the learning points in $\mathbb{R}^d$, and the linear system to solve is usually very stable and well conditioned. We never have to use the equivalent of kriging's nuggets (for some other studies, splines for up to 3000 learning points in a 17 dimension space have no problems).

For each of the three DOE, the three metamodels are built for each of the five responses. Then the metamodels are tested on two sets of 500 test points (one set is normally (Gaussian) distributed in $\mathbb{R}^{10}$, the other is uniformly distributed in $[-3 ; +3]^{10}$) to compute the Mean Square Error (MSE) between metamodel and true simulation. Some of these responses are rather smooth on most of $[-3 ; +3]^{10}$, but very stiff on a small parts of this domain.

For this case study, the results are:

<u>Comparison of DOE</u>

The comparison of the MSE with different types of DOE, metamodels, responses and test sets indicates that, generally speaking:

- the LHS DOE leads to slightly lower MSE than Halton's sequence
- Halton's sequence leads to lover MSE than the combination of classical DOE.

<u>Comparison of metamodels</u>

For metamodels, the same type of comparisons indicates that, generally speaking:

- MSE with splines are lower than with universal kriging
- MSE with universal kriging are similar or slightly lower than with ordinary kriging

Even if the MSE is usually lower with splines, the kriging packages provide additional information through the uncertainty of the surface. This information can be used to answer the problematic since we can consider the metamodel as a probabilistic function. Then we compare the percentage of compliance of the components considering the mean of the kriging response, the probabilistic kriging response and the splines surface.

In conclusion of this case study, space filling designs offer a lower MSE than the combination of composite designs. Splines seem to be more accurate on the test points, but the probabilistic information allows us to get a more reliable final result with kriging.