THE COBBLE™ ALGORITHM: MACROMODELS FOR MEMS VIA STEPWISE, SEQUENTIAL, DESIGN OF EXPERIMENTS FOR PATCHED FUNCTIONAL APPROXIMATION

Selden B. Crary^{1,2} and Khanhtran N. Phan¹

¹Center for Integrated Sensors and Circuits
The University of Michigan
Ann Arbor, Michigan 48109-2122, USA

²Center for Microinstruments
Technical University of Denmark
DK-2800, Lyngby/Copenhagen

ABSTRACT

We outline a new algorithm, COBBLE, for the generation of macromodels based on computer simulations. The algorithm uses a stepwise, sequential, design-of-experiments approach to functional approximation and is applied to a MEMS example.

INTRODUCTION

Modeling and simulation of microsensor devices and systems is essential for the understanding of device and system behavior. In previous work we have focused on applying established techniques from the branches of mathematics known as design of experiments and functional approximation. We have also extended these techniques by the development of new algorithms and software implementations, such as the I-OPT™ program that finds optimal designs for functional prediction under the I-optimality criterion, a method that is the design-of-experiments counterpart to least-squares curve fitting [1]. These methods have been successfully demonstrated on problems arising in the development of MEMS, namely the efficient calibration of sensors and the efficient functional approximation of sensor responses via finite-element analysis [2].

Recently, we have been extending these capabilities by developing a new algorithm that provides a highly efficient, sequential, design-of-computer-experiments approach to the construction of a patched functional approximation to device or system performance, as expressed by the results of simulations.

In this paper we demonstrate the application of this algorithm (named COBBLE for Computer-Based Blind Empiricism), for finding parsimonious functional approximations of a pressure-sensor device performance over a wide range of parameter values. The objective is to obviate the need for additional FEA runs by using the parsimonious models as surrogates for the FEA runs, thus dramatically reducing computational time and expense for additional runs that may be used for optimization, confirmation, or design of new devices. The challenge is to find a means to significantly reduce the number of FEA runs required for a given level of accuracy of the functional approximation, i.e., to avoid as much as possible the “curse of dimensionality” that arises in multi-parameter settings.

COBBLE

Here is how COBBLE works. As initial inputs to COBBLE, the user provides the following:

- A list of parameters and parameter ranges. The parameters may be discrete or continuous geometrical values (e.g., boss diameter, diaphragm diameter, thicknesses, etc.), material properties (anisotropic moduli of elasticity, Poisson’s ratios, etc.), or constraints as may be required by the simulator (e.g., whether or not the bending degrees of freedom of the boss are to be constrained in order to reduce computational complexity).

- A nominal run of the device or system (e.g., the output of an FEA run of the pressure sensor at nominal values of the parameters).
- A (possibly null) set of inequality constraints for the parameters (e.g., that the diameter of the boss of the diaphragm pressure sensor be less than the diameter of the diaphragm itself).
- (Optional) An educated guess as to the extent of the parameter space near the nominal starting point, over which a given degree of approximation can be expected to be valid, called a “trust region” (e.g., a second-degree approximation can be expected to be valid over a $\pm 10\%$ range of diaphragm diameters.)
- The required accuracy for the functional approximation (e.g., $\pm 3\%$ of the maximum absolute value of an output variable, such as the displacement normal to the undeflected diaphragm).

We use the Buckingham Π Theorem [3] to minimize the number of dimensionless independent variables. Then a form of optimal factor screening [4] is used to identify irrelevant variables using a small number of simulations. Also, the COBBLE algorithm extends advanced design-of-experiments methods used in physical experiments to the realm of computer experiments, with its different distributional assumptions about error, by drawing upon the work of Sacks, Schiller, and Welch [5]. In addition, the new COBBLE algorithm includes a supervisory subroutine that uses Bayesian methods to manage the tradeoffs among accuracy, time, computational cost, and choice of method of model generation.

A key ingredient of COBBLE is its use of many fewer simulations than are required in factorial designed experiments. In k dimensions, factorial methods use $(m+1)^k$ points in an m^{th} -degree functional approximation over a patch. Even if shared points among adjacent patches are considered, there are 2^k points per patch for full second-degree models. This exponential dependence on dimension can be mitigated somewhat by the use of fractional-factorial methods, but the computational explosion remains severe. By contrast, the optimal-design approach recognizes that there are only $(k+m)!/k!m!$ required points for a full m^{th} -degree approximation in each patch. With shared points this can be reduced to $(k+1)^2/2^k$ points per patch for models of second degree. For example, in three dimensions the factorial method requires eight simulations per second-degree patch, whereas the optimal-design approach requires only two. The factor of reduction of required runs grows with dimension, as shown in Figure 1. For example, with $k=10$ dimensions, the full-factorial approach requires 1024 simulations per second-degree patch, whereas the optimal-design approach requires only ~ 0.12 simulations per patch, a reduction of nearly 10^4 in the required number of simulations.

After the algorithm suggests a new set of simulation runs, the user then makes additional runs, which may include none, some, or all of those proposed by the algorithm, as well as any additional runs that the user chooses that were not suggested by

COBBLE. When these runs are completed, the user reports the parameter values and respective simulation results back to COBBLE, and the iteration cycles until COBBLE has found a patched functional approximation over the entire parameter space of interest, within the required accuracy.

Figure 1. The cobblestone efficiency grows exponentially with the number of factors.

EXAMPLE

The pressure sensor provides an example of the operation of COBBLE. First we created a parameterized FEA input file for ANSYS, our FEA software. We then sought a parsimonious model of the displacement of the diaphragm normal to the plane of the undeflected diaphragm, using the boss diameter (nominal value $R=300\mu\text{m}$) and the diaphragm diameter (nominal value $r=500\mu\text{m}$) as independent variables. The ranges of these two variables and the constraints are shown in Fig. 2, below.

Figure 2. The space of constrained independent variables, showing the initial "trust region."

After a few iterations through COBBLE and the FEA code, 16 additional runs had been made using the FEA code, and we found that a third-degree bivariate polynomial model met the accuracy requirement of $\pm 3\%$ over a rectangular region somewhat larger than, and oriented by 30% ccw with respect to the original trust region. Figure 2 shows the original trust region and the locations of the 17 FEA runs, in a plot where the independent variables have been reduced to the range $[-1,1]^2$. The curved lines denote statistically determined estimates of the boundaries of the region where the accuracy requirement is met. The rectangle oriented at approximately 30% with respect to the original trust

region is the rectangle with the maximal area that bounds a region meeting the accuracy requirements.

Figure 3. Initial trust region (dashed square) is shown again, this time in reduced variables, along with the (asymmetrical) locations of the inputs for the first 17 FEA runs. Also shown are curved boundaries for the region over which the $\pm 3\%$ accuracy requirement is estimated to hold, and the oriented rectangle with maximal area inscribed in that region.

After the nominal plus 16 additional FEA runs used for the functional approximation in the initial region, we have a statistical basis for the best local rectangular tiling, including orientation. COBBLE can then proceed to suggest input values for additional FEA runs. With sharing of points between rectangular regions, only 5 additional FEA runs per new region are necessary.

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