IDENTIFICATION OF VIRTUAL COMPUTATIONAL OBJECT'S PROPERTIES BY USING OF SCREENING DESIGNS

Jacek Pietraszek, Edward Lisowski

Krakow University of Technology
Department of Applied Informatics
Jana Pawla II Ave. 37, 31-864 Krakow, Poland
tel.: +48 12 6283580, fax: +48 12 648 82 67
e-mail: pmpietra@mech.pk.edu.pl, lisowski@mech.pk.edu.pl

Abstract

The paper presents results of investigation on the method of determination of significant properties in the case of virtual computational objects like FEM models. Typical approach is very time-consuming and involves the sequence of meshing and high performance computing. The method proposed in the paper is time-saving by utilization of the experimental design methodology, in particular the screening design analysis. The analysis based on Plackett-Burman designs and fractional factorial designs is focused on the maximum cost reduction. It provides to the main effects analysis. In the mentioned case of the virtual computational object it allows determining significant properties of the model and to focus on the selected most important parameters affecting the key properties of the object. Time-saving is obtained by eliminating insignificant factors from the study area. The mathematical basis for this approach is well known from the experimental design area, and the novelty is the use of it to the particular deterministic computational object. Specific metrics are defined for approximation accuracy, computational cost and their relationship to show the benefits of the method. Identification was carried out in two ways. The first method is used when the two elements are available: the set of output feature values obtained experimentally and chosen error criterion for comparing the predicted and measured values of output characteristics. The second method requires a binding equation or equations, which must be satisfied.

Keywords: *modelling, screening design, effects analysis*

1. Introduction

Continuously increasing of modern processors' computing power and capacity of operating memory are the reason of more detailed and precise computational models, and the reason of their increasing complexity. Because of that complexity, simulation research of computational models is more and more resource and time consuming. One of the fundamental element of the investigation is to estimate the sensibility of the selected model's property related to small changes of its significant parameters and then to order these parameters according to descending influence on the investigated property.

In traditional approach it is provided by identification of the first-order derivatives of the selected property with respect to analyzed parameters i.e. by evaluation of the property's gradient. The symmetric finite difference scheme is typically involved to evaluate the gradient and (2n+1) star points are required, where n is a number of analyzed model's parameters. The relationship of the number of points from the number of parameters is linear, what is already very favourable in view of the cost calculation, but it appears that it is possible to further reduce the number of points with the method proposed in the design of experiment methodology [1]. This way the information is obtained at significantly reduced workload.

2. Proposed method of procedure

The method described below is a general outline of the proposal dealt with computational models as objects of research and utilization of screening experimental designs (Plackett-Burman and fractional factorial) to identify and rank the value of the average effects. These in turn will help to determine these parameters which are the most affecting the results obtained from the model. The set of test function was used during the verification of the proposed approach. The functions were used as examples of the computational models. A large set of multidimensional test points was constructed randomly in the domain of the test function and then each point was used as a centre point for a locally settled experimental design. Next, the outcome of the test function was identified for all cases of experimental design as a simulated equivalent of measurement process. For the given outcome values, the linear model of main effects was identified and the values of the effects were determined. Simultaneously, the estimates of first order derivatives were evaluated for the design's centre points basing on the finite difference scheme and the main effects were evaluated alternatively. Supplementary, the derivatives were evaluated analytically from the gradient of the test function and the main effects were evaluated in the third way. The comparative analysis was made with the values of the effects.

2.1. Description of the investigated object

The computational model is a mapping, which forecasts values of some properties of the physical object basing on the values of other properties of the object. It may symbolically express by formula (1):

$$\mathrm{M} : \mathbf{P} \rightarrow \mathbf{C}\,, \tag{1}$$

where:
M - mapping being the computational model,
P - the set of input variables (factors) of the model,
C - the set of output properties of the model.

The cardinality of **P** set depends on the level of model's details. This set contains parameters describing modelled object, its environment and parameters describing the model itself (2):

$$\mathbf{P} = \mathbf{P}_{\mathrm{O}} \times \mathbf{P}_{\mathrm{M}}\,, \tag{2}$$

where:
$\mathbf{P}_{\mathrm{O}}$ – the set of parameters describing properties of the physical object and its environment,
$\mathbf{P}_{\mathrm{M}}$ – the set of parameters describing properties of the model (e.g. number of mesh's nodes).

Determination of the appropriate values for $\mathbf{P}_{\mathrm{M}}$ parameters proceeds in the model's identification process. Identification is carried out in two ways. The first method is used when the two elements are available: the set of output feature values obtained experimentally and chosen error criterion for comparing the predicted and measured values of output characteristics. The method is based on to minimize the error criterion in the space of model parameters (3):

$$\mathrm{F}_1(\mathrm{c}_{\mathrm{exp}}, \mathrm{M}(\mathrm{p}_{\mathrm{O}}, \mathrm{p}_{\mathrm{M}})) \xrightarrow[\mathrm{p}_{\mathrm{M}}]{} \min\,, \tag{3}$$

where:
F_1 - error criterion to minimize,
$\mathrm{c}_{\mathrm{exp}}$ - output values obtained experimentally,
M - the mapping representing the computational model,
p_{O} - values of the parameter describing properties of the physical object and its environment,
p_{M} - values of the parameters describing model's properties.

The second method requires a binding equation or equations, which must be satisfied. Normally this is to minimize some criterion of error dependent on residuals of binding equations (4) in the space of model's parameters:

$$\mathrm{F}_2(\mathrm{p}_{\mathrm{O}}, \mathrm{p}_{\mathrm{M}}, \mathrm{M}(\mathrm{p}_{\mathrm{O}}, \mathrm{p}_{\mathrm{M}})) \xrightarrow[\mathrm{p}_{\mathrm{M}}]{} \min\,, \tag{4}$$

where:
F_2 - error criterion to minimize,
M - the mapping representing the computational model,

p_O - values of the parameters describing properties of the physical object and its environment,
p_M - values of the parameters describing model's properties.

This way is characteristic, among others, for FEM models, where a typical task for the assumed loads shall designate a field of stresses and strains.

2.2. The identified model

As a basis for further work a linear model of main effects was assumed [1] (5):

$$c_{ME}(b_0, b_i, p_i) = b_0 + \sum_{i=1}^{n} b_i p_i \ , \tag{5}$$

where:

c_{ME} - the model of main effects forecasting the selected output property of the analyzed computational model,
b_0 - the intercept of the main effects model,
b_i - coefficient of the main effects model associated with the *i*-th input parameter,
p_i - *i*-th input parameter of the analyzed computational model,
n - number of input parameters included in the calculation model.

In this way the model (5) becomes a local approximation of the analyzed computational model (1) after proper identification of the coefficients.

2.3. Test functions

Analysis was conducted using two test functions: Rastrigin's and Trid. These functions are representative of a wider group of so called difficult functions used to test different optimization techniques.

Rastrigin's function provides the features of the object without interaction between the input variables. The original form defined for two variables was given by Rastrigin in 1974 [4], widely propagated in 1989 by Törn and Zilinskas [5], and then in 1991, generalized to the case of multi-dimensional by Mühlenbein, Schomisch and Born [3]. A model function (6) is defined for any number of independent variables, and the domain (7) is a fixed size hyper-cube:

$$c_R(n, p_i) = 10n + \sum_{i=1}^{n} (p_i^2 - 10\cos(2\pi p_i)) \ , \tag{6}$$

$$-5.12 \le p_i \le 5.12 \quad i = 1 \ldots n \ , \tag{7}$$

where:

c_R - Rastrigin's function simulating the computational object,
n - number of input parameters of computational object,
p_i - *i*-th input parameter of the computational object.

Trid function being modification of the tridiagonal Broyden function [2] provides characteristics of object having interactions between the input variables. A function formula (8) is defined for any number of independent variables, and the domain (9) is hyper-cube of variable size depending on the number of input parameters:

$$c_T(p_i) = \sum_{i=1}^{n} (p_i - 1)^2 - \sum_{i=2}^{n} p_i p_{i-1} \ , \tag{8}$$

$$-n^2 \le p_i \le n^2 \quad i = 1 \ldots n \ , \tag{9}$$

where:

c_T - Trid function simulating computational model,
n - number of input parameters of the computational model,
p_i - i-th input parameter of the computational model.

2.4. Comparative measures

The result of computations is vectors of the effects evaluated for each input parameter of the model. The effect is defined as the difference in response for the opposed values of the analyzed parameter, with the average settings of other parameters. In the case of the main effects model (5), this takes the form of equation (10):

$$\mathrm{Eff}_{\mathrm{DOE}\,i}=\mathrm{c}_{\mathrm{ME}}\begin{pmatrix}\hat{\mathrm{p}}_j=0\\ \hat{\mathrm{p}}_i=+1\end{pmatrix}-\mathrm{c}_{\mathrm{ME}}\begin{pmatrix}\hat{\mathrm{p}}_j=0\\ \hat{\mathrm{p}}_i=-1\end{pmatrix},\quad i=1\ldots n,\ j=1\ldots(i-1),(i+1)\ldots n, \tag{10}$$

where:

c_{ME} - the main effects model (5), by which the effect of *i*-th parameter is calculated,

$\hat{\mathrm{p}}_i$ - *i*-th parameter coded according to DOE methodology,

$\mathrm{Eff}_{DOE\ i}$ - absolute effect calculated for the *i*-th parameter.

In the case of the traditional difference scheme, it is a two-point system, where the effect is directly determined as the difference of responses (11) of the analyzed computational model (1) for the next and previous node:

$$\mathrm{Eff}_{\mathrm{Trd}\,i}=\mathrm{c}\begin{pmatrix}\mathrm{p}_j=\mathrm{xc}_j\\ \mathrm{p}_i=\mathrm{xc}_i+\mathrm{h}_i\end{pmatrix}-\mathrm{c}\begin{pmatrix}\mathrm{p}_j=\mathrm{xc}_j\\ \mathrm{p}_i=\mathrm{xc}_i-\mathrm{h}_i\end{pmatrix},\quad i=1\ldots n,\ j=1\ldots(i-1),(i+1)\ldots n, \tag{11}$$

where:

c - analyzed computational model,

xc_{j} - real (uncoded) centre value of the *i*-th parameter,

h_j - real (uncoded) value corresponding to the difference between an encoded value and 0 for the *j*-th parameter; the traditional nomenclature is the star arm length of the finite difference star scheme.

$\mathrm{Eff}_{Trd\ i}$ - absolute effect evaluated by finite difference for the *i*-th parameter.

In the case of an analytical gradient test function effect is calculated as twice the differential for the corresponding increment of the parameter (12):

$$\mathrm{Eff}_{\mathrm{Grd}\,i}=2\mathrm{h}_i\left.\frac{\partial \mathrm{c}_{\mathrm{Test}}(\mathrm{p})}{\partial \mathrm{p}_i}\right|_{p_j=xc_j}\quad i,\ j=1\ldots n\,, \tag{12}$$

where:

c_{Test} - considered test function,

xc_{j}, h_j - definitions same as for formula (11),

$\mathrm{Eff}_{Grd\ i}$ - absolute effect calculated using the analytical gradient for the *i*-th parameter.

The effects of individual input parameters may have different values, and thus differences in their values calculated by different methods may vary in the magnitude. To avoid the influence of scale and masking smaller effects by larger, the standardization of the individual values of individual effects was adopted. The components of effects were standardized individually related to the components of the reference vector. The effects vector calculated by traditional finite difference method was assumed as reference. Standardization for the effects calculated by DOE method is given by formula (11):

$$\mathrm{Eff}_{std\ DOE\ i}=\frac{\mathrm{Eff}_{DOE\ i}}{\mathrm{Eff}_{Trd\ i}}\quad i=1\ldots n\,, \tag{11}$$

where:

$\mathrm{Eff}_{\mathrm{std\ DOE}\ i}$ - effect calculated for the *i*-th parameter by experimental design, standardized with respect to effect based on finite difference,

$\mathrm{Eff}_{\mathrm{DOE}\ i}$ - absolute effect calculated for the *i*-th parameter by experimental design,

$\mathrm{Eff}_{\mathrm{Trd}\ i}$ - absolute effect calculated for the *i*-th parameter by finite difference scheme.

The same standardization was carried out with respect to the vector calculated by the differential effects and supplied a vector with all components equal to value 1 (12):

$$\mathrm{Eff}_{std\,Trd\,i} = 1 \quad i = 1\ldots n. \tag{12}$$

The measure D_1 of the difference between two vectors of effects is defined as dimensionless quotient of the Euclidean length of the standardized effects vector and the length of the reference vector (13):

$$D_1 = \frac{\sqrt{\sum_{i=1}^{n}\left(\mathrm{Eff}_{std\,DOE\,i} - \mathrm{Eff}_{std\,Trd\,i}\right)^2}}{\sqrt{\sum_{i=1}^{n}\mathrm{Eff}_{std\,Trd\,i}^{\;2}}}. \tag{13}$$

Due to property (12) relationship (13) can be presented in a simplified form (14):

$$D_1 = \frac{\sqrt{\sum_{i=1}^{n}\left(\mathrm{Eff}_{std\,DOE\,i} - 1\right)^2}}{\sqrt{n}}. \tag{14}$$

This measure provides information about the difference between the results obtained from two different methods (proposed and traditional) on the basis of data available only by numerical observation and the absence of information about the analytical form of the actual mapping of the investigated object.

A similar measure and the standardization procedure may be performed in case of acceptance (in the formula (11)) as a vector of reference results calculated from the gradient (12). A standardization formula then becomes (15):

$$\mathrm{Eff}_{std\,2\,DOE\,i} = \frac{\mathrm{Eff}_{DOE\,i}}{\mathrm{Eff}_{Grd\,i}} \quad i = 1\ldots n, \tag{15}$$

where:

$\mathrm{Eff}_{std2\,DOE\,i}$ - effect calculated for the *i*-th parameter using experimental design, standardized with respect to the effect calculated from the gradient,

$\mathrm{Eff}_{DOE\,i}$ - absolute effect calculated for the *i*-th parameter using experimental design,

$\mathrm{Eff}_{Grd\,i}$ - absolute effect calculated for the i-th parameter using analytical gradient.

The measure D_2 of the difference between two vectors of effects is defined as dimensionless quotient of the Euclidean length of the standardized effects vector and the length of the reference vector (gradient-based vector of effects) (16):

$$D_2 = \frac{\sqrt{\sum_{i=1}^{n}\left(\mathrm{Eff}_{std\,2DOE\,i} - 1\right)^2}}{\sqrt{n}}. \tag{14}$$

This measure provides information about the difference between the results obtained from the proposed method and actual properties of the investigated object (the test function in such case).

3. Results of numerical studies

3.1. Studied experimental designs

Experimental design listed in Tab. 1. were admitted to the numerical studies. These designs vary depending on the number of input factors. It should be noted, that Plackett-Burman designs are the most appropriate solution only for certain numbers of factors, while in other cases, more cost-effective is the use of fractional factorial designs.

Tab. 1. Experimental designs used for calculation

No.	Number of factors	Number of runs	Number of runs (traditional)	Symbol	Description
1.	2	4	5	2**2	full factorial design
2.	3	4	7	2**(3-1)	fractional factorial design
3.	4	8	9	2**(4-1)	fractional factorial design
4.	11	12	23	P-B n=12	Plackett-Burman design

3.2. The results obtained for Rastrigin's test function

The base for numerical studies was experimental designed, listed in Tab.1. The population of 1000 centre points was randomly generated in the domain of the Rastrigin's test function. As the spread of the experimental design (coded values -1 and +1), the ranges 10%, 20% and 30% were assumed related to the size of the Rastrigin's test function domain. The means, medians and quantiles 0.975 for D_1 and D_2 distributions were empirically determined for generated experimental designs. The results obtained for D_2 are presented in Tab. 2. The values obtained for D_1 have magnitude 10^{-12} and thus have been omitted.

3.3. Results obtained for Trid test function

The base for numerical studies was experimental designs listed in Tab.1. The population of 1000 centre points was randomly generated in the domain of the Trid test function. As the spread of the experimental design (coded values -1 and +1), the ranges 1%, 2% and 3% were assumed related to the size of the Trid test function domain. The means, medians and quantiles 0.975 for D_1 and D_2 distributions were empirically determined for generated experimental designs. The results obtained for D_1 are presented in Tab. 3. and for D_2 in Tab. 4.

Tab. 2. Descriptive statistics of D_2 for the object simulated by Rastrigin's function

Descriptive statistics	Design range		
	10%	20%	30%
i = 2, design: full factorial 2**2			
Mean	0.020	0.090	0.210
Median	0.017	0.066	0.144
0.975 quantile	0.058	0.297	0.610
i = 3, design: fractional factorial 2**(3-1)			
Mean	0.023	0.092	0.193
Median	0.017	0.066	0.144
0.975 quantile	0.044	0.261	0.529
i = 4, design: fractional factorial 2**(4-1)			
Mean	0.030	0.116	0.219
Median	0.017	0.067	0.149
0.975 quantile	0.106	0.250	0.718
i = 11, design: Plackett-Burman n=12			
Mean	0.022	0.091	0.204
Median	0.017	0.067	0.146
0.975 quantile	0.063	0.365	0.720

Tab. 3. Descriptive statistics of D_1 for the object simulated by Trid function

Descriptive statistics	Design range		
	10%	20%	30%
i = 2, design: full factorial 2**2			
Mean	~10^{-13}	~10^{-13}	~10^{-13}
Median	~10^{-13}	~10^{-13}	~10^{-13}
0.975 quantile	~10^{-13}	~10^{-13}	~10^{-13}
i = 3, design: fractional factorial 2**(3-1)			
Mean	0.029	0.066	0.099
Median	0.011	0.024	0.032
0.975 quantile	0.189	0.457	0.606
i = 4, design: fractional factorial 2**(4-1)			
Mean	0.020	0.034	0.046
Median	0.004	0.009	0.013
0.975 quantile	0.085	0.153	0.255
i = 11, design: Plackett-Burman n=12			
Mean	0.093	0.170	0.283
Median	0.029	0.059	0.087
0.975 quantile	0.725	1.182	2.228

Tab. 4. Descriptive statistics of D2 for the object simulated by Trid function

Descriptive statistics	Design range		
	10%	20%	30%
i = 2, design: full factorial 2**2			
Mean	~10^{-13}	~10^{-13}	~10^{-13}
Median	~10^{-13}	~10^{-13}	~10^{-13}
0.975 quantile	~10^{-13}	~10^{-13}	~10^{-13}
i = 3, design: fractional factorial 2**(3-1)			
Mean	0.031	0.082	0.120
Median	0.011	0.023	0.035
0.975 quantile	0.158	0.686	0.853
i = 4, design: fractional factorial 2**(4-1)			
Mean	0.022	0.033	0.043
Median	0.004	0.008	0.013
0.975 quantile	0.138	0.168	0.328
i = 11, design: Plackett-Burman n=12			
Mean	0.084	0.173	0.234
Median	0.028	0.055	0.084
0.975 quantile	0.517	1.442	1.551

3.4. Discussion of results

The results obtained using experimental designs can be regarded as being fully compatible with the differential scheme in the absence of interaction between the parameters of the computational model. In the presence of interactions there are differences, whose size is strongly dependent on the spread of the experimental design. Differences are acceptable in the case of small spreads. This means that if one uses screening experimental designs to determine the effects, the spread of the design should be rather small and the exact ranges shall be determined individually.

4. Conclusions

The results obtained with the proposed method are fully consistent with the traditional method for the object without interaction parameters, or similar in the case of object with the interaction of parameters. The benefits from the proposed method increases with the number of parameters describing considered computational object. The accuracy of the proposed method depends on the spread of the used experimental design i.e. size of design space. The spread of experimental design should be adjusted individually to the problem.

References

[1] Montgomery, D. C., *Design and Analysis of Experiments*, Wiley, New York 1997.
[2] Moré, J. J., Garbow, B. S., Hillstrom, K. E., *Algorithm 566: FORTRAN Subroutines for Testing Unconstrained Optimization Software*, ACM Trans. Math. Software, 7(1), 136-140, 1981.
[3] Mühlenbein, H., Schomisch, D., Born, J., *The Parallel Genetic Algorithm as Function Optimizer*, Parallel Computing, Vol. 17, No. 6,7, 619-632, 1991.
[4] Rastrigin, L. A., *Extremal Control Systems*, Znanie-Sila, Moscow 1974.
[5] Törn, A., Zilinskas, A., *Global optimization*, LNCS 350, 1-255, Springer-Verlag, New York 1989.