AN SURROGATE BASED OPTIMIZATION ALGORITHM FOR NONLINEAR CONSTRAINED OPTIMIZATION AND ITS APPLICATIONS TO STRUCTURAL OPTIMIZATION

Henry Cortés, hcortes@optimize.ufrj.br
José Herskovits, jose@optimize.ufrj.br
COPPE/Federal University of Rio de Janeiro - Caixa Postal 68503 - Rio de Janeiro, Brazil

Andrés Tovar, atovarp@unal.edu.co
National University of Colombia - Cr. 30 45-03, Edif. 453, Of. 401 - Bogotá, Colombia

Abstract. *Surrogate-based optimization (SBO) methods are frequently employed in engineering design optimization of complex systems by replacing complete numerical models. Their use is convenient in the case of numerical models built with experimental data, models in which the analysis or sensitivity analysis is very expensive, models with discontinuous derivatives or with no available derivatives, and very complex optimization problems. The methodology commonly employed for optimal design with surrogated models is usually iterative. It begins by defining an initial approximated model (surrogate model) that is optimized by the algorithm, then a new model is constructed in the approximated optimum previously obtained. This procedure is repeated until a stopping criterion is satisfied. The main drawbacks of this approach include the inability to prove global convergence, the oscillation, in practice, of intermediate solutions, and the difficulty in obtaining feasible designs. The purpose of this investigation is to obtain a rigorous feasible point optimization technique for nonlinear constrained optimization, which would ensure global convergence. In practice, this means that all intermediate designs are feasible and the objective function is reduced at every iteration. In this contribution the surrogates are linear programs. Instead of using the optimum of the surrogates as a new design, a search direction is defined and a line search is performed to decrease the objective function. The proposed algorithm is applied to shape optimization of two-dimensional elastic structures. The sensitivity analysis are avoided and the numerical results are encouraging.*

Keywords: *Optimization Methods, Shape Optimization, Mathematical Programming, Metamodelling, Surrogate Based Optimization (SBO)*

1. INTRODUCTION

Surrogate-based optimization (SBO) has been shown to be an effective approach for the design of computationally expensive models such as those found in the design of automotive, aerospace and consumer products. Frequently, single discipline simulations used for analysis are being coupled together to create complex coupled simulation systems, it is the case of multidisciplinary design optimization (MDO) problems. The computational cost of executing a single complex simulation makes these problems very expensive for optimization, so the algorithms of direct optimization are rarely used. As solution to this problem are required approximated models with low computational cost (known as *surrogate models* or *metamodels*). The approximated models are based on limited number of calls to the high fidelity models. Once constructed, the substitute model (*surrogate*) can substitute the exact original model for optimization purposes.

In some cases, the engineer has to design under a time constraint and therefore the optimization process may be terminated prematurely. In this case an algorithm that provides a feasible design at each iteration would be desirable.

The methodology commonly employed for optimal design with surrogate models is usually sequential. The basic concept is to apply nonlinear optimization to the minimization of an local or global approximation of the objective function and constraints. The approximations implemented could be any of a wide range of models (metamodels). Once built the metamodel or surrogate model, it is included on the original problem providing second order information (in the case of Taylor series approximations) or substituting entirely that functions. Then is solved an minimization subproblem of the approximations. The process continue with the construction of new approximations or upgrading they and following again the same scheme until attain a condition of finalization.

Optimization methods employing approximation models was originated since 1970's (Schmit Jr. and Miura 1976) and have become more popular within the engineering community. Numerous surveys of these methods exist (Barthelemy and Haftka 1993; Sobieszczanski-Sobieski and Haftka 1997).

The models used for approximation can be classified basically under two criteria related to the response approximation. According the *number of points* in the design space included at the simulation, can be of *one point* or of *multiple points.* According the *scope* of the approximation, can be *local* or *global* depending if are made for represent a part of the design space or all him.

There are too other kind of methods that instead of approximating the original response, approximate the subproblem response, one example of this kind of techniques are called *multilevel optimization* (Sobieski 2000).

Figure 1 shows a general review of the main approximation methods in optimization, illustrating its corresponding classification.

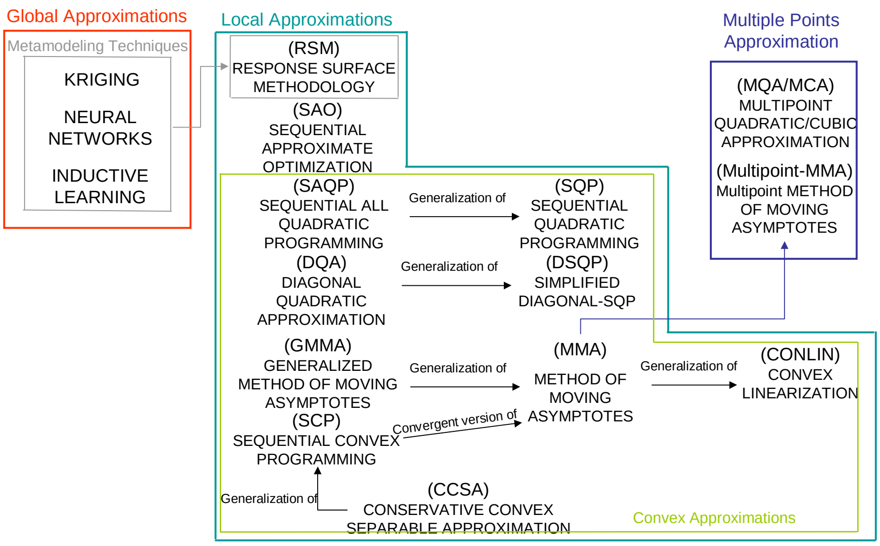


Figure 1. Main Approximation Methods in Optimization

2. SURROGATE-BASED OPTIMIZATION (SBO)

Surrogate-based optimization (SBO) methods have become established as effective techniques for engineering design problems through their ability to tame non-smoothness and reduce computational cost.

A number of surrogate model selections are possible. First, the surrogate may be of the *data fit* type, which is a non-physics-based approximation typically involving interpolation or regression of a set of data generated from the original model. Data fit surrogates can be further characterized by the number of data points used in the fit, where local approximations (e.g., first or second-order Taylor series) use data from a single point, multipoint approximations (e.g., two-point exponential approximations (Fadel and Barthelemy 1990) (TPEA) or two-point adaptive nonlinearity approximations (Xu and Grandhi 1998) (TANA)) use a small number of data points often drawn from the previous iterates of a particular algorithm, and global approximations (e.g., polynomial response surfaces, kriging, neural networks, radial basis functions, splines) use a set of data points distributed over the domain of interest, often generated using a design of computer experiments. A second type of surrogate is the *model hierarchy* type (also called multifidelity, variable fidelity, etc.). In this last case, a model is still physics-based but is of lower fidelity (e.g., coarser discretization, reduced element order, relaxed solver tolerances, omitted physics) is used as the surrogate in place of the high-fidelity model. A third type of surrogate model involves *reduced-order modeling* techniques such as proper orthogonal decomposition (POD) in computational fluid dynamics or spectral decomposition in structural dynamics. These surrogate models are generated directly from a high-fidelity model through the use of a reduced basis and projection of the original high-dimensional system down to a small number of generalized coordinates. These surrogates are still physics-based (and may therefore have better predictive qualities than data fits), but do not require multiple system models of varying fidelity (as required for model hierarchy surrogates).

The general nonlinear optimization problem is

$$\begin{cases} \min\limits_{x} & f(x) \\ \text{s. t.} & g_i(x) \leq 0; i = 1, 2, \ldots, m \\ & h_i(x) = 0; i = 1, 2, \ldots, p \\ & x_l \leq x \leq x_u, \end{cases} \tag{1}$$

where $x \in \mathbb{R}^n$ is the vector of design variables, and f, g and h are smooth functions in $\mathbb{R}^n$ and at least one of these functions is nonlinear. The corresponding surrogate-based optimization (SBO) algorithm may be formulated in several ways. In all cases, SBO solves a sequence of k approximate optimization subproblems; however, many different forms of the surrogate objectives and constraints in the approximate subproblem can be explored (Eldred and M. 2006). In particular, the subproblem objective may be a surrogate of the original objective or a surrogate of a merit function (most commonly, the Lagrangian or augmented Lagrangian), and the subproblem constraints may be surrogates of the original constraints, linearized approximations of the surrogate constraints, or may be omitted entirely. Each of these combinations is shown in Tab. 1, where black indicates an inappropriate combination, gray indicates an acceptable combination, and blue indicates a common combination (Eldred and M. 2006).

Table 1. SBO approximate subproblem formulations.

	Original Objective	Lagrangian	Augmented Lagrangian
No constraints			TRAL
Linearized constraints		SQP-FDIPA*	
Original constraints	Direct surrogate		IPTRSAO

*Technique presented by the authors

In Tab. 1, the approach in the row 1, column 3 is known as the trust-region augmented Lagrangian (TRAL). While this approach was provably convergent, convergence rates to constrained minima have been observed to be slowed by the required updating of Lagrange multipliers and penalty parameters (Pérez and Watson 2004). Prior to converging these parameters, SBO iterates did not strictly respect constraint boundaries and were often infeasible. A subsequent approach (IPTRSAO (Pérez and Watson 2004)) that sought to directly address this shortcoming added explicit surrogate constraints (row 3, column 3 in Tab. 1).

While this approach does address infeasible iterates, it still shares the feature that the surrogate merit function may reflect inaccurate relative weighting of the objective and constraints prior to convergence of the Lagrange multipliers and penalty parameters. That is, one may benefit from more feasible intermediate iterates, but the process may still be slow to converge to optimality. The concept of this approach is similar to that of SQP-like SBO approaches (Alexandrov and Newman 2000) which use linearized constraints.

In that the primary concern is minimizing a composite merit function of the objective and constraints, but under the restriction that the original problem constraints may not be wildly violated prior to convergence of Lagrange multiplier estimates. Here, the merit function selection of the Lagrangian function is most closely related to SQP, which includes the use of first-order Lagrange multiplier updates that should converge more rapidly near a constrained minimizer than the zeroth-order updates used for the augmented Lagrangian.

The SQP-Feasible Directions Interior Point Algorithm (SQP-FDIPA)(row 2, column 2 in Tab. 1) presented by the authors is also related to SQP. Where subproblems (Quadratic Programs) define a feasible descent direction, and the feasible solutions are guaranteed on each iteration due the inclusion of the real constraints in the line search. Here the first order information is obtained from a data fit model (Response Surface) on each iteration.

All of these previous constrained SBO approaches involve a recasting of the approximate subproblem objective and constraints as a function of the original objective and constraint surrogates. A more direct scheme has been termed the direct surrogate approach since it optimizes surrogates of the original objective and constraints (row 3, column 1 in Tab. 1) without any recasting. It is attractive both from its simplicity and potential for improved performance.

On each of the k iterations in the SBO strategy, an step is predicted along a descent direction $d^k := (x - x^k)$ or within a trust region. This completes an SBO cycle, and the cycles are continued until either soft or hard convergence criteria are satisfied.

3. SURROGATE-BASED FEASIBLE DIRECTIONS INTERIOR POINT ALGORITHM

Sequential Quadratic Programming (SQP), that is at the moment the largest employed method for nonlinear constrained optimization, is a quasi-Newton technique based on an idea proposed by Wilson (Wilson 1963) and interpreted by Beale (Beale 1967).

A *Quadratic Program* is a class of constrained optimization problems such that the objective is a convex quadratic function and the constraints are linear. Efficient techniques to solve this problem are available, even when inequality constraints are included. The exact solution is obtained after a finite number of iterations (Luenberger 1984). To solve the problem

$$\begin{cases} \min_{x} \quad f(x) \\ \text{s. t. } g(x) \leq 0 \\ \qquad h(x) = 0, \end{cases} \tag{2}$$

Wilson proposed to define the search direction d and new estimates of the Lagrange multipliers λ and μ by solving at each iteration

$$\begin{cases} \min_{d} \quad \frac{1}{2} d^T B d + \nabla f^T(x) d \\ \text{s. t. } \nabla g^T(x) d + g(x) \leq 0 \\ \qquad \nabla h^T(x) d + h(x) = 0. \end{cases} \tag{3}$$

Since the quadratic programming problem 3 is a convex problem (quadratic programm with $d \in \mathbb{R}^n$ as unknown) based on Taylor series approximations for the objective (quadratic approximation) and the constraints (linear approximation), the global minimum satisfies the Karush-Kuhn-Tucker optimality conditions.

Wilson's is a Newton algorithm. Garcia Palomares and Mangasarian proposed later a quasi-Newton technique (Garcia Palomares and Mangasarian 1976), Han obtained a globally convergent algorithm (Han 1977) and Powell proved superlinear convergence (Powell 1978).

An exact penalty function is taken as the objective of the line search.

In Sequential Quadratic Programming algorithms, the matrix S is defined as a quasi-Newton approximation of the Hessian of the Lagrangian. Most of the optimizers employ the following BFGS rule modified by Powell:

Let be $\delta = td$ and $\gamma = \nabla_x L(x + td, \lambda_0) - \nabla_x L(x, \lambda_0)$.

$$B := B + \frac{\gamma\gamma^T}{\delta^T\gamma} - \frac{B\delta\delta^T B}{\delta^T B\delta}. \tag{4}$$

The asymptotic speed of convergence has similar properties as quasi-Newton algorithms for equality constrained optimization and Maratos' effect can also occur.

Feasible directions algorithms are an important class of methods for solving constrained optimization problems. At each iteration, the search direction is a feasible direction of the inequality constraints and, at the same time, a descent direction of the objective or an other appropriate function. A constrained line search is then performed to obtain a satisfactory reduction of the function without loosing the feasibility.

The fact of giving feasible points makes feasible directions algorithms very efficient in engineering design, where functions evaluation is in general very expensive. Since, any intermediate design can be employed, the iterations can be stopped when the cost reduction per iteration becomes small enough.

There are also several examples that deal with an objective function, or constraints, that are not defined at infeasible points. This is the case of size and shape constraints in structural optimization. When applying feasible directions algorithms to real time problems, as feasibility is maintained and cost reduced, the controls can be activated at each iteration.

Taking into account the previous considerations, an algorithm of feasible directions based on SQP is a very good choice as an efficient and robust optimization approach. However, the approximations in Taylor series expansion used and it mathematical demonstration are based on the suppose of *smooth functions*, which is not the case in many engineering problems. Also, frequently the function derivatives are no available or its calculations are very expensive.

Following these reasoning, the algorithm developed on this investigation follow the idea of the SQP feasible directions algorithm developed by Herskovits in (Herskovits 1983) and by Herskovits and Carvalho in (Herskovits and Carvalho 1986), where the first order information is obtained of the metamodel acquired by *data fit* using constrained least squares (attaining the consistency requirement), i.e. based on the Response Surface Methodology (RSM)(Myers R. H. 1995; Simpson and Allen 2001).

Algorithm: Surrogate-Based Feasible Directins Interior Point Algorithm

Parameters: $r > 0$, $\varphi > 0$ and $\alpha \in (0, 1)$.

Data: Initialize $x \in \mathbb{R}^n$ feasible.

STEP 1. Obtain the surrogates and its corresponding derivatives.

Solve the following linear constrained least square problems for the objective and each constraints respectively.

$$\begin{cases} \min\limits_{b} \ \ \|Xb - c\|_2 \\ \text{s. t. } \hat{f}(x) = f(x). \end{cases} \tag{5}$$

Where $X \in \mathbb{R}^{ne \times (n+1)}$ is the matrix of the levels of the design variables ($x_i, i = 1, \ldots, n$) in the *least squares normal equations* notation; ne is the number of objective function evaluations required to make the fit; $b \in \mathbb{R}^{(n+1)\times 1}$ is the vector of the regression coefficients, and $c \in \mathbb{R}^{ne \times 1}$ is the vector with the response value, that is, $c_i = f(x_i)\ \forall x_i \in E(x) := \{x \cup Rand(ne, x, r)\}$, where

$Rand(ne, x, r)$ is a set compound by ne random points generated within a neighborhood of half size r and center x, i. e., space filling experiment.

$$\hat{g}(x) = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_n x_n \qquad \text{is the linear model for each constraint.} \tag{6}$$

$$\hat{f}(x) = b_0 + \sum_{j=1}^{n} b_j x_j + \sum_{j=1}^{n} b_{jj} x_j^2 + \sum\sum_{i<j} b_{ij} x_i x_j \tag{7}$$

$$\equiv \frac{1}{2} x^T \hat{S} x + \tilde{f}^T x + f_0 \qquad \text{is the quadratic model for the objective function,} \tag{8}$$

$$\text{where } \ \hat{S} \ \text{ is the approximated Hessian of } \ f. \tag{9}$$

STEP 2. Computation of a descent direction d_0 and an estimate of the Lagrange multipliers λ_0.

Solve the quadratic program in d_0

$$\begin{cases} \min\limits_{d_0} \ \ \frac{1}{2} d_0^T \hat{B} d_0 + \nabla \hat{f}^T(x) d_0 \\ \text{s. t. } \nabla \hat{g}^T(x) d_0 + g(x) \leq 0 \end{cases} \tag{10}$$

STEP 3. Computation of the search direction d (feasible and descent).

i) Let the active set be $J(x) \stackrel{\text{def}}{=} \{j \in 1, 2, \ldots, m \mid \lambda_{0j} > 0\}$ and
$g_J(x) \stackrel{\text{def}}{=} [g_j(x)]^T, j \in J(x)$.
If $g_J^T(x)[\nabla \hat{g}_J^T(x) \hat{B}^{-1} \nabla \hat{g}_J(x)]^{-1} e < 0$, find

$$\rho_J = \frac{(1-\alpha) \nabla \hat{L}^T(x, \lambda_0) d_0}{g_J^T(x)[\nabla \hat{g}_J^T(x) \hat{B}^{-1} \nabla \hat{g}_J(x)]^{-1} e} \tag{11}$$

where the Lagrangian $L^T(x, \lambda) = f(x) + \lambda^T g(x)$ and $e \stackrel{\text{def}}{=} [1, 1, \ldots, 1]^T$

ii) Let the inactive set be $\overline{J}(x) \stackrel{\text{def}}{=} \{j \in 1, 2, \ldots, m \mid \lambda_{0j} = 0\}$.
For each $j \in \overline{J}(x)$, if

$$\{\nabla \hat{g}_j^T(x) \hat{B}^{-1} \nabla \hat{g}_J(x) [\nabla \hat{g}_J^T(x) \hat{B}^{-1} \nabla \hat{g}_J(x)]^{-1} e - 1\} < 0,$$

find

$$\rho_j = \frac{g_j(x) + \nabla \hat{g}_j^T(x) d_0}{\nabla \hat{g}_j^T(x) \hat{B}^{-1} \nabla \hat{g}_J(x) [\nabla \hat{g}_J^T(x) \hat{B}^{-1} \nabla \hat{g}_J(x)]^{-1} e - 1}. \tag{12}$$

iii) Set $\rho = inf\{\varphi\|d_0\|^2, \rho_J, \rho_j, j \in \overline{J}(x)\}$.

iv) Solve the quadratic program in d

$$\begin{cases} \min\limits_{d} \ \frac{1}{2}d^T\hat{B}d + \nabla\hat{f}^T(x)d \\ \text{s. t. } \nabla\hat{g}_J^T(x)d + g_J(x) = -\rho e \end{cases} \tag{13}$$

STEP 4. Line search.

Find a step length t satisfying a given constrained line search criterion on the Lagrangian function $L(x, \lambda_0)$ and such that $(x + td)$ is a feasible point of the exact nonlinear program.

STEP 5. Update: $\hat{B}$ (the approximated Hessian of the Lagrangian), and x.
Let be $\delta = td$ and $\gamma = \nabla_x\hat{L}(x + td, \lambda_0) - \nabla_x\hat{L}(x, \lambda_0)$.

i) If $\delta^T\gamma < 0.2\delta^T\hat{B}\delta$, then compute

$$\phi = \frac{0.8\delta^T\hat{B}\delta}{\delta^T\hat{B}\delta - \delta^T\gamma}$$

and set $\gamma = \phi\gamma + (1 - \phi)\hat{B}\delta$.

ii) Set

$$\hat{B} := \hat{B} + \frac{\gamma\gamma^T}{\delta^T\gamma} - \frac{\hat{B}\delta\delta^T\hat{B}}{\delta^T\hat{B}\delta}$$

and

$$x := x + td$$

STEP 6. Go back to Step 1.

4. EXAMPLES OF APPLICATIONS

The following examples have been performed implementing the surrogate-based interior point algorithm in the Matlab® program.

4.1 Barnes test problem

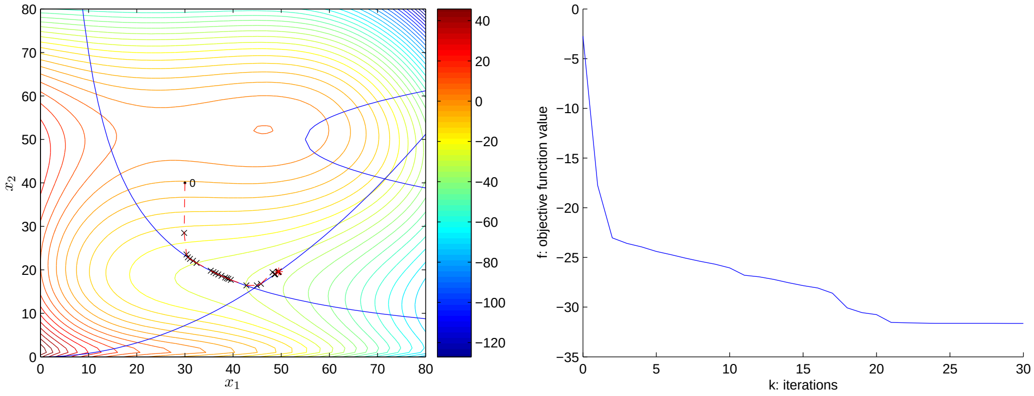
The Barnes problem (Wujek 1997) is a test problem with two continuous design variables and three nonlinear inequality constraints.

Starting from the feasible point (30,40) the algorithm converge to a local minimizer in 30 iterations, it is, the same order of iterations that the derivatives enhanced version (using exact derivatives for both objective and constraints).

The Fig. 2(a) show the contour plot for the Barnes function. The Fig. 2(b) show the convergence of the algorithm to the local minimizer with decrement of the objective function value in each iteration (no oscillates are present).

4.2 Structural shape optimization of a bracket

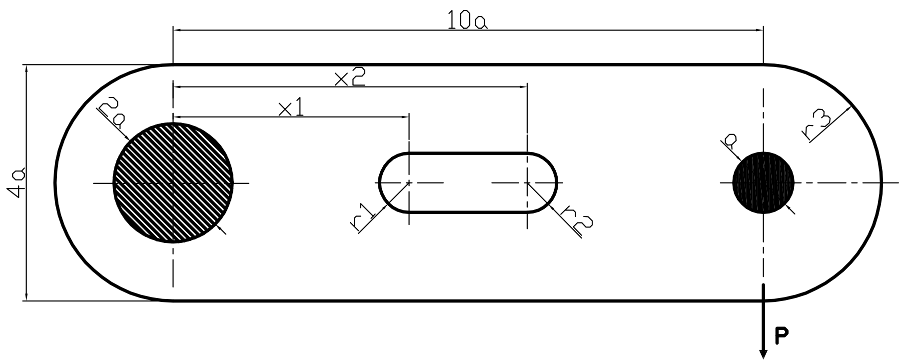
Figure 3 shows geometry and the design parametrization, and response analysis results for a bracket problem. A total of five design variables ($x = [r1, r2, r3, x1, x2]$) have been selected to change the inner/outer boundary of the bracket, while maintaining symmetry. The plane stress formulation is used with a thickness of 0.004 m. The bracket is made of steel with $E = 200$ GPa, and $\nu = 0.33$. The force applied is $P = 6 \times 10{-}3$ MN, and the magnitude of $a = 0.02$ m.



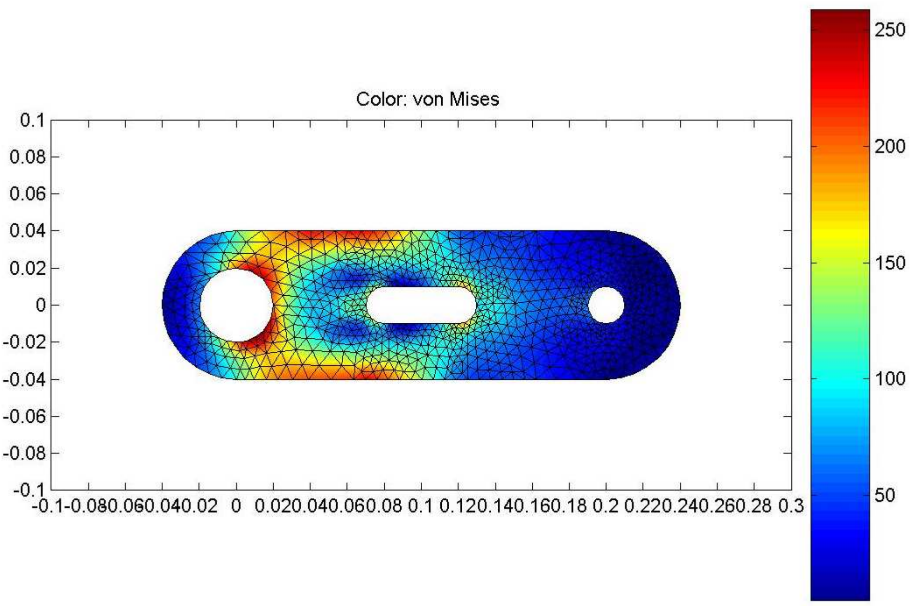
(a) Contour plot of function

(b) Convergence

Figure 2. Results for the Barnes function using SBO with the SQP-FDIPA.



(a) Problem definition.



(b) Initial FEA result. von Mises Stress in MPa.

Figure 3. Geometry, design variables, and finite element analysis result of bracket.

The structural shape optimization problem is formulated in such a way that the total volume of the structure is minimized with respect to its shape design variables, with design constraints defined as the von Mises stress, as

$$\begin{cases} \min\limits_{x} \quad Vol.(x) \\ \text{s. t. } \sigma_{MAX} \leq 350\, MPa \end{cases} \tag{14}$$

The optimization problem converged in fourth iterations. Figure 4 shows the analysis results at the optimum design.

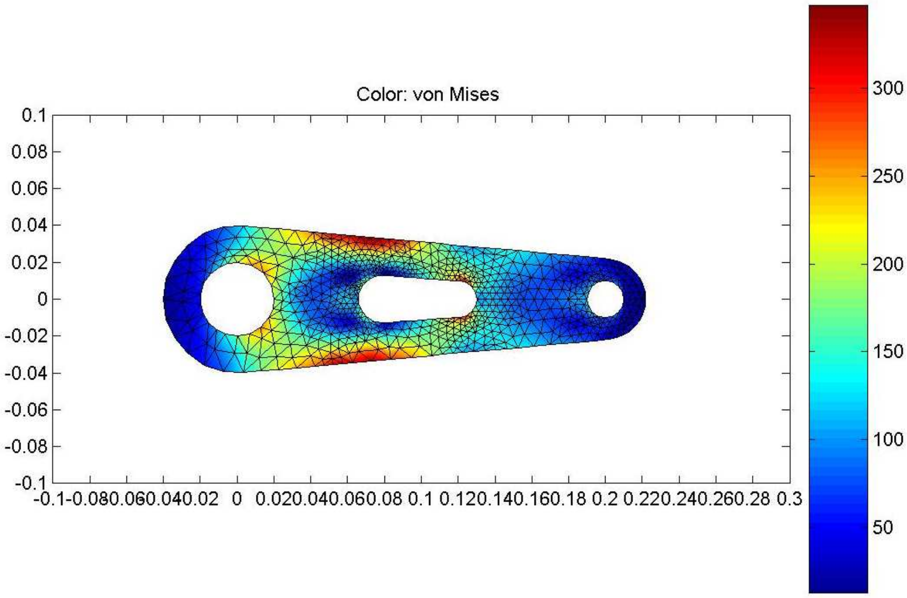


Figure 4. Analysis result at optimum design. von Mises stress in MPa.

Optimal volume is reduced from 7.3382×10^{-5} m^3 to 5.10083×10^{-5} m^3. A total of 92 response analyses were carried out during the fourth optimization iterations. When FEM is used with re-meshing precess (quadratic triangular elements).

5. CONCLUSIONS

This research present a new algorithm based on approximation ideas which make use of the efficiency and robustness of the SQP approach in a version more attractive for the engineering field which enables the capability of generate feasible points and always decrease the objective avoiding oscillate.

Other capabilities was included from the surrogate-based ideas such as the possibility of lead with non-smooth functions and, work with experimental data.

Our approximation in all senses (Taylor series expansion in the SQP, and data fit for the surrogate model) are local, and the algorithm presented on this investigation converge to a local minima.

Our results are encouraging, mainly in fields with few design variables (e. g. Shape Structural Optimization), because the high number evaluations of the real function to minimize the variance of the model due to data fit adjust required to guaranty minimal variance in the model.

Future works could be the use of other scheme that allow many more design variables without decrease the quality of the approximation.

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