Preprint of a manuscript submitted to:
Compumag 2007, Aachen

Simulation-based design improvement of a superconductive magnet by mixed-integer nonlinear surrogate optimization

T. Hemker, O. von Stryk, H. De Gersem, and T. Weiland

The numerical optimization of continuous parameters in electrotechnical design using electromagnetic field simulation is already standard. In this paper, we describe a new sequential surrogate optimization approach for simulation-based mixed-integer nonlinear programming problems. We apply the method for the optimization of combined integer- and real-valued geometrical parameters of the coils of a superconductive magnet.

1 Introduction

For the numerical solution of simulation-based optimization problems, especially as occurring in engineering design, surrogate optimization has demonstrated besides random search and sampling methods to provide powerful methods for overcoming the specific difficulties involved. Typically, simulation codes are included as black box objective function generators, which may require much computational time for function evaluation, but usually do not provide any gradient information as it is required by efficient mathematical optimization methods. Furthermore, iterative, or heuristic methods, or low-order approximations of tabular data, or other kinds of numerical methods underlying the simulation code result in noisy objective function evaluations, which rule out the application of Newton-type, or other gradient-based methods, if the gradients are estimated by standard finite differences. If in addition, the optimization variables include integer-valued variables the problem complexity grows even further. Even when stated in analytical formulation mixed-integer nonlinear programs (MINLP) are challenging optimization problems. Although MINLPs receive which received more and more attention from the optimization community, in the context of simulation-based optimization only computationally expensive random search methods like genetic algorithms are currently known in the engineering community.

For the case considered in this paper the homogeneity of the magnetic field in the aperture of a superconductive magnet is determined by the geometry of the coil (Fig. 1). Especially the position of the coil blocks and the number of turns in each coil block are influencing the quality of the aperture field. The layout of the coils has to obey mechanical constraints such as, e.g., a minimal distance between two adjacent coil blocks. Invoking a separate real-valued optimization for every possible distribution of the integer number of turns over the coil blocks is not feasible. Hence, a constrained, mixed-integer nonlinear optimization has to be carried out.

2 Surrogate optimization for mixed-integer nonlinear problems

2.1 Optimization problem formulation

For a chosen design determined by variables $p \in \mathrm{IR}^{n_p}$ and $s \in \mathrm{IN}^{n_s}$ the objective function value evaluated through magnetic field simulation has to be minimized:

$$\min_{(p,s)\in\Omega} f(p,s).$$

The parameter settings for p and s are supplied to the simulation which returns the resulting objective function value $f(p,s)$. The feasible domains Ω for (p,s) is bounded by box and linear constraints to meet the geometric requirements of the magnet design. These are given by $A(p,s)^T \leq b^T$, with $b \in \mathrm{IR}^{n_b}$ and a matrix $A \in \mathrm{IR}^{n_b \times (n_p+n_s)}$, where n_p, n_s, and n_b describe the dimensions of p, s and b.

2.2 Modeling of a surrogate problem

We use an extension as it is proposed in [1] to the classical approach from Sacks et al. [2] known as Design and Analysis of Computer Experiments (DACE) to handle not only continuous, real-valued variables but also discrete, integer-valued ones in such a way that the simulation-based objective function is approximated by a stochastic model. For a given set of feasible system designs $\mathcal{B} = \{(p_i, s_i)\}_{i=1,\dots,n}$ and the simulation outputs $f(p_i, s_i)$ the surrogate function $\hat{f}$ build by DACE has to meet

$$f(p_i, s_i) = \hat{f}(p_i, s_i), \quad \forall \quad (p_i, s_i) \in \mathcal{B}.$$

An underlying stationary Gaussian stochastic process with a constant mean is assumed to determine $\hat{f}$ and the DACE parameters are estimated by a maximum likelihood estimation as originally proposed in [2]. The main effects of f should be covered by $\hat{f}$,

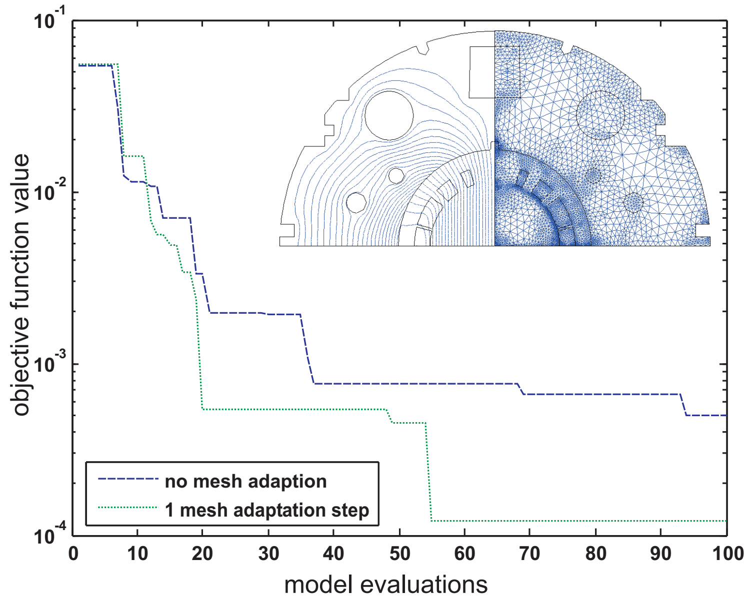

Figure 1: Convergence of the optimization process with respect to the number of model evaluations, magnetic flux lines and adapted finite-element mesh of the magnet model.

but it is obvious that $\hat{f}$ is exact only on $\mathcal{B}$. The expected mean square error (MSE) that is calculated during the modeling process provides a measure for prediction of the approximation quality of $\hat{f}$.

2.3 Solving a surrogate problem

The modeling of a surrogate problem carries out a computational cheap and completely analytically given surrogate function for the optimization that is defined on a completely real-valued domain $\hat{\Omega}$, the continuous relaxation of Ω. Thus, the use of decomposition methods developed for MINLP like branch and bound (BB) [3] is enabled. These can normally not be applied for the original objective function, because the underlying simulations are often not defined for the relaxed integer-valued variables. Furthermore, the noise induced by the numerical simulation into the original objective function is smoothed out, and thereby the step by step generated BB-tree of NLP subproblems can be solved efficiently by sequential quadratic programming methods [4]. This also allows us to include the explicitly given linear and box constraints directly into the surrogate problem formulation.

2.4 Sequential optimization procedure

The often limited, available computational power requires to avoid the simulation of a spacefilling set of possible system designs at once. This suggests a more efficient sequential optimization procedure. First a small initial set of system designs $\mathcal{B}_{in} = \{(p_l, s_l)\}_{l=1,\ldots,k}$ is selected and simulated to generate an initial surrogate optimization problem. To start the iteration we add the minimizer (p^{*in}, s^{*in}) of the initial surrogate problem as the next candidate which is evaluated by the electromagnetic field simulation and added to $\mathcal{B}_{in}$ to become a new basis $\mathcal{B}_1$ of a new surrogate function $\hat{f}_1$. This is repeated in each iteration to build new surrogate problems by extending the previous basis. But if a minimizer (p^{*j}, s^{*j}) during iteration j is inside an ϵ-ball, around the elements of $\mathcal{B}_j$, the process is forced to find a design (p^{MSE*j}, s^{MSE*j}), which maximizes the MSE of $\hat{f}_j$ in order to get more information about unexplored areas of $\hat{\Omega}$, respectively Ω. Another effect of this switching criteria is that the optimization can not stuck into a local minimum. The described procedure ensures that all earlier obtained information as computational expensive simulation output is included for the selection of new promising designs during the iterative approximation and optimization procedure. This is done until a stopping criteria is satisfied, in our case after a limited number of objective function evaluations by the underlying simulation.

3 Numerical results

The described approach is implemented using MATLAB and a DACE toolbox [5], combined with an electro-magnetic field simulation software [6]. For a fixed number of four coil blocks we optimize the design by continuous variation of the position vector $p \in \mathbb{R}^3$, and the vector of numbers of turns $s \in \mathbb{N}^3$. One initial expert's guess, and two random chosen feasible system designs form the initial basis $\mathcal{B}_{in}$. The quality improvement of the magnetic field according to the applied number of simulation calls is illustrated in Fig. 1. The numerical simulation of the system design is as a start applied for the optimization process without mesh adaptation, and a second time with one mesh adaptation step. It turns out that the best found designs of all applied optimization methods without mesh adaptation are unstable with regard to small changes in the positions of the coil blocks, which indicates the necessity of a mesh adaptation. But for both settings an expected aperture field quality is reached with less than 100 simulation calls, which is 2 to 3 times less compared to further approaches with evolutionary algorithms optimizing just the real-valued variables of this design problem.

4 conclusion

Using the presented surrogate optimization approach to determine the coil geometry the aperture field quality of the considered superconductive magnet can be significantly improved consuming a small number of computational expensive electromagnetic field simulations only.

References

[1] Hemker, Fowler, and von Stryk, "Derivative-free optimization methods for handling fixed costs in optimal groundwater remediation design," in *Proc. of the CMWR XVI - Computational Methods in Water Resources*, 19-22 June 2006.

[2] Sacks, Schiller, and Welch, "Design for computer experiments," *Technometrics*, vol. 31, pp. 41–47, 1989.

[3] Grossmann, "Review of nonlinear mixed-integer and disjunctive programming techniques," *Optimization and Engineering*, vol. 3, pp. 227–252, 2002.

[4] Gill, Murray, and Wright, "SNOPT: An SQP algorithm for large-scale constrained optimization," *SIAM Review*, vol. 47, pp. 99–131, 2005.

[5] Lophaven, Nielsen, and Sondergaard, "DACE, a matlab kriging toolbox," IMM, Tech. Rep. IMM-TR-2002-12, August 2002.

[6] Pahner, Mertens, De Gersem, Belmans, and Hameyer, "A parametric finite element environment tuned for numerical optimization," *IEEE Trans. Magn.*, vol. 34, no. 5, pp. 2939–2939, Sept. 1998.