A PARALLEL AUTOMATIC SIMULATION TOOL FOR CAVITY SHAPE OPTIMIZATION*

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Abstract

We present a parallel automatic shape optimization workflow for designing accelerator cavities. The newly developed 3D parallel optimization tool Opt3P based on discrete adjoint methods is used to determine the optimal accelerator cavity shape with the desired spectral response. Initial and updated models, meshes and design velocities of design parameters for defining the cavity shape are generated with Simmetrix tools for mesh generation (MeshSim), geometry modification and query (GeomSim), and user interface tools (SimModeler). Two shape optimization examples using this automatic simulation workflow will be presented here. One is the TESLA cavity with higher-order-mode (HOM) couplers and the other is a superconducting rf (SRF) gun. The objective for the TESLA cavity is to minimize HOM damping factors and that for the SRF gun to minimize the surface electric and magnetic fields while maintaining its operating mode frequency at a prescribed value. The results demonstrate that the automatic simulation tool allows an efficient shape optimization procedure with minimal manual operations. All simulations were performed on NERSC supercomputer Cori system for solution speedup.

INTRODUCTION

Simulations play an important role in the design and optimization of accelerator cavities and components. The use of automated optimization techniques to improve cavity designs will result in significant cost savings and performance improvements for accelerator applications. However, usually optimizing cavity geometry subject to various design criteria is performed manually and the optimized design is achieved by the expertise of the designer. Optimization codes that exist are hard to use especially for complicated 3D geometries when one has to deal with changes of design parameters and the updates of the model and the subsequent mesh at each iteration of the optimization procedure.

At the time when computing power keeps on increasing through parallel computation, an automatic cavity optimization code, Opt3P, has been developed in ACE3P [1, 2] which is an advanced multiphysics parallel simulation suite, including integrated electromagnetic, thermal, and mechanical solvers, developed by researchers at the SLAC National Accelerator Laboratory. Opt3P, incorporating advanced geometry properties computation and mesh adaptation with respect to changes in design parameters, will definitely relieve designers from spending the time on laborious manipulations and free them up for more creative thinking to come up with a better design.

CAVITY SHAPE OPTIMIZATION

PDE Constrained Optimization

A shape optimization based on the adjoint method has been implemented in ACE3P's frequency-domain eigensolver module Omega3P [3, 4], which calculates the electromagnetic properties of resonant modes in an accelerator cavity. One critical step in the optimization cycle (see Fig. 1) is to calculate the design velocity field ($\partial x_r/\partial d_j$) – the motion of each mesh surface node due to a change in each design variable. Analytic expressions for design velocities can be derived for simple geometric shapes. However, for complex 3D geometric entities, one used to have to resort to moving the mesh surfaces by hand to evaluate the design velocity, which requires code implementation whenever a new structure optimization is done. In this work we developed a general approach to calculating the design velocity. providing a fully automatic shape optimization procedure. In the following, we will describe the major components that have been implemented in Opt3P optimization workflow.

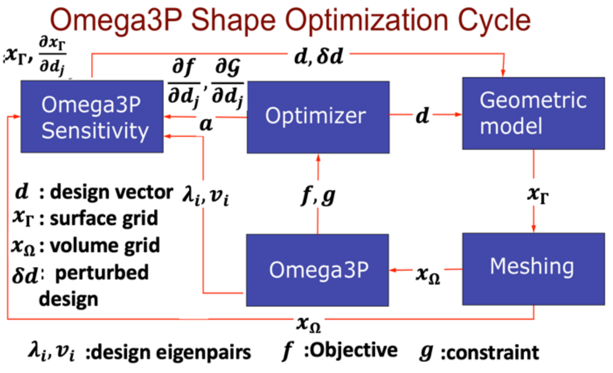

Figure 1: Flow chart for adjoint optimization method.

Objective Functions for Cavity Shape Optimization

The optimization objectives with constraints for accelerator cavity shape optimization can be categorized in the following: 1) Maximize the shunt impedance of the operating mode; 2) Minimize external quality factors of higher-order-modes (HOM); 3) Minimize surface electric or magnetic field on cavity wall; 4) Constrain the operating mode

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frequency to a certain value; 5) Specify power coupling factor of the operating mode to a certain value; 6) Specify field profile across cells in a multi-cell cavity.

To accommodate a general approach of defining various objective functions with their design gradients, a substantial part of the optimization code has been developed with clear class hierarchies within the framework of ACE3P.

Mesh Generation and Geometry Modification

For each optimization step, it is necessary to create a mesh that reflects the updated geometry. The starting point is the change to the set of design parameters as requested by Opt3P. Simmetrix's tools [5] take that information and update the geometry accordingly. Next, Simmetrix's tools can automatically determine the portions of the mesh/model where mesh motion can be used to update the mesh instead of completely remeshing the geometry. The functionality has been integrated into Opt3P and includes a step to curve the mesh so it conforms better to the geometry for use with ACE3P.

Design Velocity Computation

The optimization procedure needs to calculate shape sensitivities which require design velocities on boundary surfaces. The needed derivatives are calculated using automatic differentiation for a variety of model modifications. Examples are geometry changes due to translations/rotations/scaling, shape parameter modifications, (e.g. changes in path and profile for swept surfaces), or where geometry is defined through a constraint, relating geometric objects with each other. The derivatives are evaluated at the locations of the mesh vertices and exported. In Opt3P we have developed mesh data structures with the inclusion of design velocity and implemented functions to read in the design velocities. All these functions are implemented in parallel to reduce possible computational bottlenecks in the simulation workflow.

Automatic Optimization Workflow

A python script has been written to execute the overall optimization procedure as shown in Fig. 2. Users can modify the design parameters and visualize the changes to the geometry by using SimModeler GUI and then execute this python script to perform the optimization procedure automatically.

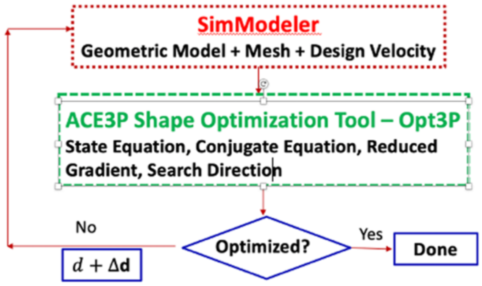

Figure 2: Workflow of the overall optimization procedure.

APPLICATIONS

In the following, we demonstrate two applications using automatic optimization workflow.

Peak Surface Field Optimization in SRF Cavity

Fig. 3 is the model of a realistic cavity design of a superconducting rf (SRF) gun, based on a recent design developed at University of Wisconsin. The objective is to minimize the surface electric field at the nose cone iris and the surface magnetic field at the left top corner of the cavity wall while maintaining the operating mode frequency at 200 MHz. For simplicity, the four design parameters are shown in Fig. 3. This is essentially a 2D optimization problem. A major challenge in the optimization procedure is to calculate the design velocity at the locations to handle the tangential intersections of the line with the circular and elliptical shapes. SimModeler calculates the design velocity using automatic differentiation carried through a Newton-Raphson iteration to solve for the tangent point when the design parameters defining the radii of the ellipses change.

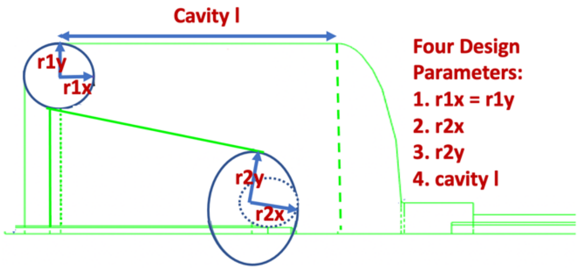

Figure 3: A CAD drawing of SRF gun and definition of design parameters.

As an illustration, the objective to minimize the surface electric field while maintaining the accelerating mode frequency at 200 MHz can be expressed by the cost function

$$F = w_1 |E_p| + w_2 \frac{|f - f_0|}{f_0} \qquad (1)$$

where E_p is the peak surface field evaluated by its L_p norm defined as

$$|E_p| = \left(\frac{\int |E|^p \, d\Gamma}{\int d\Gamma} \right)^{\frac{1}{p}} \qquad (2)$$

Here f and f_0 are the accelerating mode and the target frequency, respectively. Thus, the cost function, Eq. (1), consists of a design objective and a constraint whose magnitudes are controlled by the weight functions w_1 and w_2, respectively. Note that when p goes to infinity, the L_p norm approaches the peak value on the surface of interest. L_p is chosen to be 64 for this investigation, which is large enough to estimate the peak field. In practice, L_p will be increased in the optimization procedure to ensure convergence.

For simplicity, we minimize only the peak surface electric field on the circular surface created by r2y and r2x (r2y = r2x) by varying the two design parameters Cavity_l and r2x described in Fig. 3. The optimization procedure as a function of iteration number is shown in Fig. 4. It can be seen that the peak electric field is reduced while the frequency reaches the target value. Fig. 5 shows the shape change artificially enlarged by 10 times for visualization purpose.

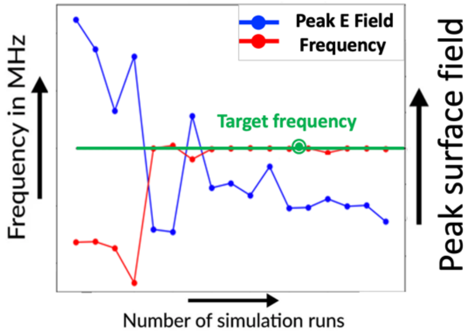

Figure 4: Peak surface electric field optimization.

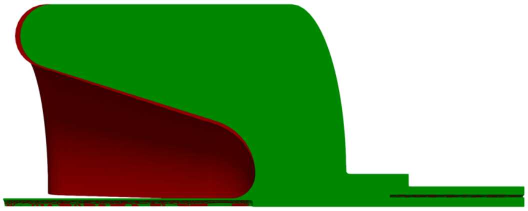

Figure 5: Cavity shape before (Green) and after (Red, enlarged) optimization.

External Q Optimization for Higher Order Modes in TESLA Cavity

The TESLA cavity with higher-order-mode (HOM) couplers was used for demonstration of optimizing 3D complex geometry structure. The CAD model of the TESLA cavity is shown in Fig. 6. The design parameters describing component movements are shown in Fig. 7.

There are several objectives that the optimum shape of the cavity must achieve to meet the design requirements. The following test provides minimized external Q value of HOM's, specifically the two dipole modes at frequency $f = 1.73$ GHz with high external Q. The objective is to minimize $^{\lambda_r}/_{\lambda_i}$, where λ_r and λ_i are the real and imaginary parts of the eigenvalues obtained by solving a complex eigenproblem using Omega3P, which arises from the damping coaxial ports at the HOM couplers.

Figure 8 shows the external Q value changes from running automatic optimization workflow using two active design parameters: angle of HOM tank about z-axis and loop angle in the HOM tank about z-axis. Convergence is achieved after a few iterations. Three meshes are shown with different colors to illustrate the component locations at different iterations of the optimization process.

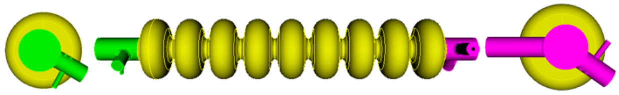

Figure 6: TESLA cavity with HOM couplers.

Figure 7: Design parameters for the TESLA cavity.

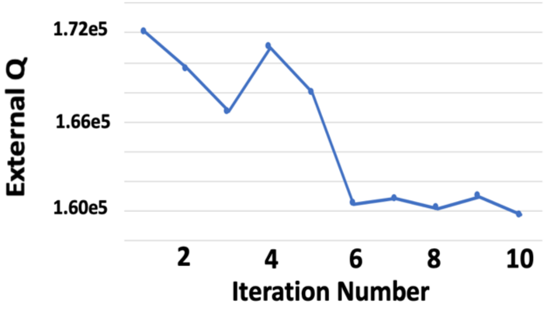

Figure 8: External Q convergence.

SUMMARY

An automatic shape optimization workflow has been developed through integrating Simmetrix's geometry and meshing tools that provides initial and updated models, meshes and design velocities of design parameters for defining the cavity shape with ACE3P optimization module Opt3P. The whole workflow has been successfully performed for optimizing realistic cavities using parallel computation on NERSC computing resources, which enables the normal lengthy optimization procedure to exploit the computation power of supercomputers.

ACKNOWLEDGEMENT

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REFERENCES

[1] L. Xiao, L. Ge, Z. Li, and C.-K. Ng, "Advances in Multiphysics Modeling for Parallel Finite-Element Code Suite ACE3P," *IEEE J. Multiscale Multiphys. Comput. Tech.*, vol. 4, p. 298, 2019. `doi: 10.1109/JMMCT.2019.2954946`

[2] K. Ko and A. E. Candel, "Advances in Parallel Electromagnetic Codes for Accelerator Science and Development", in *Proc. LINAC'10*, Tsukuba, Japan, Sep. 2010, paper FR101, pp. 1028-1032.

[3] V. Akcelik, L.-Q. Lee, Z. Li, C. Ng, L. Xiao, and K. Ko, "Large scale shape optimization for accelerator cavities," *J. Phys.: Conf. Ser.*, vol. 180, p. 012001, 2009.

[4] V. Akelik, K. Ko, L.-Q. Lee, Z. Li, C.-K. Ng, and L. Xiao, "Shape determination for deformed electromagnetic cavities," *J. Comp. Physics*, vol. 227, pp. 1722–1738, 2008. `doi:10.1016/j.jcp.2007.09.029`

[5] Simmetrix, Inc., `http://www.simmetrix.com/`, 10 Executive Park Dr., Clifton Park, NY 12065.