Large scale shape optimization for accelerator cavities

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Abstract. We present a shape optimization method for designing accelerator cavities with large scale computations. The objective is to find the best accelerator cavity shape with the desired spectral response, such as with the specified frequencies of resonant modes, field profiles, and external Q values. The forward problem is the large scale Maxwell equation in the frequency domain. The design parameters are the CAD parameters defining the cavity shape. We develop scalable algorithms with a discrete adjoint approach and use the quasi-Newton method to solve the nonlinear optimization problem. Two realistic accelerator cavity design examples are presented.

1. Introduction

Computer science research and algorithm development are crucial for the advancement of accelerator R&D. Simulation plays an important role in the design of accelerators because of its impact on performance improvement and cost reduction. However, traditional trial and error approaches are expensive and time consuming even with the help of computing. We use PDE constrained optimization techniques to provide a more efficient and effective method for the shape design of accelerating cavities. The objective is to determine the best design parameters giving the cavity shape with the desired spectral response. The constraint is the large scale Maxwell eigenvalue problem. In the following, we first discuss the discrete adjoint methods used in the shape optimization algorithm. Then, we present two realistic examples: optimization of the choke-mode cavity and the crab cavity.

2. Maxwell eigenvalue shape optimization

We consider the Maxwell eigenvalue shape optimization problem with the following form

\[
\begin{align*}
\text{minimize} \quad & J(e_i, k_i, d) \\
\text{subject to} \quad & Ke_i + jk_i We_i - k_i^2 Me_i = 0 \\
& e_i^H Me_i = 1 \\
& \Re(e_i) e_i^T M3(e_i) = 0 \\
& 1 \leq d \leq u
\end{align*}
\]

where \( e_i \in \mathbb{C}^{n_e} \) and \( k_i \) are discrete eigenvector and eigenvalues for the \( i^{th} \) mode, \( n_e \) is the number of degrees of freedom, \( d \) is the design variable vector, \( j \) is the complex number,
\( \mathbf{K}, \mathbf{M}, \mathbf{W} \in \mathbb{R}^{n_e \times n_e} \) are the stiffness, mass and waveguide matrices, \( \mathbf{e}_i^H \) is the complex conjugate transpose of \( \mathbf{e}_i \), \( \mathbf{1} \) and \( \mathbf{u} \) are the lower and upper bounds for the design variable \( \mathbf{d} \) [1]. Equations 2 and 3 are the normalization conditions. \( \Re(\mathbf{e}_i) \) and \( \Im(\mathbf{e}_i) \) are real and complex parts of eigenvector \( \mathbf{e}_i \). The objective function \( J \) may include more than one eigenmode.

To derive the optimality conditions we introduce the following Lagrange multipliers: adjoint vectors \( \mathbf{t}_i \in \mathbb{C}^{n_e} \), and adjoint constants \( \xi_i \in \mathbb{R} \) and \( \eta_i \in \mathbb{R} \). Taking inner products of the constraints with the adjoint variables we obtain the real valued Lagrangian functional:

\[
\mathcal{L}(\mathbf{e}, \mathbf{k}, \mathbf{t}, \xi, \eta, \mathbf{d}) = J + \sum_{i=1}^{n_a} \left[ \frac{1}{2} \mathbf{t}_i^H (\mathbf{K} \mathbf{e}_i + j \mathbf{k}_i \mathbf{W} \mathbf{e}_i - k_i^2 \mathbf{M} \mathbf{e}_i) + \frac{1}{2} \text{c.c.} \right.
\]

\[
+ \frac{1}{2} \xi_i \left( \mathbf{e}_i^H \mathbf{M} \mathbf{e}_i - 1 \right) + \eta_i \Re(\mathbf{e}_i)^T \mathbf{M} \Im(\mathbf{e}_i) \right] \quad (5)
\]

where c.c. is the complex conjugate of the previous term.

**Optimality Conditions.** The first order optimality conditions require stationary Lagrangian with respect to its arguments [2, 3, 4]. These variations result in the state, adjoint and inversion equations. The state equation is the forward Maxwell eigenvalue problem (Equations 1-3). The adjoint equations are obtained by taking variations of Lagrange multipliers with respect to the state variables \( \mathbf{e} \) and \( \mathbf{k} \) for each mode:

\[
\mathbf{Kt} + (jk)^* \mathbf{Wt} - (k^2)^* \mathbf{Mt} + \xi_i \mathbf{Me} + j \eta_i \mathbf{Me}^* = \frac{\partial J}{\partial \mathbf{e}}
\]

\[
j \mathbf{t}^T \mathbf{We}^* + 2k^* \mathbf{t}^T \mathbf{Me}^* = \frac{\partial J}{\partial \mathbf{k}}
\]

Adjoint equations are linear system of equations. Each mode involved in the objective function yields one adjoint equation. To obtain the design equation, we take variation with respect to the \( p \)th component of the design variable and obtain the expression for the \( p \)th component of the design equation:

\[
\frac{\partial \mathcal{L}}{\partial d_p} = \frac{\partial J}{\partial d_p} + \sum_{i=1}^{n_a} \left[ \frac{1}{2} \mathbf{t}_i^H \left( \frac{\partial \mathbf{M}}{\partial d_p} \mathbf{e}_i + j \mathbf{k}_i \frac{\partial \mathbf{W}}{\partial d_p} \mathbf{e}_i - k_i^2 \frac{\partial \mathbf{K}}{\partial d_p} \mathbf{e}_i \right) + \frac{1}{2} \text{c.c.} \right.
\]

\[
+ \frac{1}{2} \xi_i \mathbf{e}_i^H \frac{\partial \mathbf{M}}{\partial d_p} \mathbf{e}_i + \eta_i \mathbf{Re}(\mathbf{e}_i)^T \frac{\partial \mathbf{M}}{\partial d_p} \Im(\mathbf{e}_i) \right]
\]

Given a shape estimate \( \mathbf{d} \), to compute the reduced gradient we solve the state and adjoint equations, and evaluate the inversion equation. We use a quasi-Newton method to find the optimum shape and to solve the nonlinear optimization problem [5].

3. **Shape optimization for choke-mode cavity**

The first shape optimization application is the design of choke-mode cavity. This structure is an example of damped accelerator cavities proposed for high gradient accelerator research. In this design the accelerating mode is trapped inside the cavity by means of a choke structure while unwanted higher-order-modes (HOM) are coupled out from the cavity through radial waveguides and absorbed in matched loads. There are several objectives that the optimum shape of the choke-mode cavity has to achieve:

- Meet the accelerating mode frequency to 11.424 GHz.
• Satisfy field flatness for the accelerating mode.
• Maximize external Q value of the accelerating mode.
• Minimize external Q value of the higher-order-modes.
• Constrain the $\frac{R}{Q}$ (shunt impedance) of the accelerating mode.

In the design of the choke-mode cavity, the accelerating model and 18 higher-order-modes are used for optimization. Design parameters have simple bound constraints and the objective function is formulated to satisfy the required objectives. The CAD model of the choke-mode cavity with the definition of design variables are shown in Figure 1. The cavity consists of 9 cells, and the 7 center cells are required to be identical. The optimization problem has 21 design parameters. We use a penalty method to enforce the eigenvalue constraint for the accelerating mode. The nonlinear problem is solved using a quasi-Newton method with active set strategy.

![Figure 1. CAD model of the choke-mode cavity (left), and definition of design parameters for the choke-mode cavity (right).](image)

The resulted optimum design parameters are tabulated in Table 1. In addition, the HOM frequency spectrum for the initial and optimum cavities, and Q values are presented in Table 2. The original and optimum cavities are shown in Figure 2. In conclusion, shape optimization decreases Q values of higher-order-modes in the choke-mode structure considerably while the accelerating frequency is fixed at 11.424 GHz with the desired field flatness is satisfied and the $\frac{R}{Q}$ value is constrained.

| Cell 1 | Δ r1 | Δ r2 | Δ r3 | Δ r4 | Δ z1 | Δ z2 | Δ z3 |
|--------|------|------|------|------|------|------|------|
|        | 592  | -1040| -308 | 0.2  | 1696 | 590  | 445  |

| Cell 2-8 | Δ r1 | Δ r2 | Δ r3 | Δ r4 | Δ z1 | Δ z2 | Δ z3 |
|----------|------|------|------|------|------|------|------|
|          | 712  | -1712| 1410 | -157 | 1794 | 634  | 4    |

| Cell 9 | Δ r1 | Δ r2 | Δ r3 | Δ r4 | Δ z1 | Δ z2 | Δ z3 |
|-------|------|------|------|------|------|------|------|
|       | 0.7  | -1107| 207  | -192 | 1800 | 1081 | 1797 |
Table 2. Frequency and Q values for the original and optimized cavity.

| Mode number | Original Frequency | Original Q-value | Original $\frac{R}{Q}$ | Optimized Frequency | Optimized Q-value | Optimized $\frac{R}{Q}$ |
|-------------|-------------------|-----------------|----------------------|---------------------|------------------|----------------------|
| 1           | 14892740171       | 305.55          | 330                  | 14978085631         | 42.16            | 534                  |
| 2           | 14937523596       | 253.10          | 115                 | 15035058182         | 36.12            | 949                  |
| 3           | 15005849652       | 190.64          | 3553                | 15144908731         | 28.89            | 3320                 |
| 4           | 15088362142       | 135.78          | 221                 | 15172877655         | 17.79            | 894                  |
| 5           | 15172741072       | 95.86           | 17808               | 15343691411         | 24.40            | 2833                 |
| 6           | 15246074352       | 70.55           | 27920               | 14519190264         | 7.57             | 18793                |
| 7           | 15299862686       | 56.13           | 12930               | 14528647324         | 7.55             | 111636               |
| 8           | 15332802296       | 48.62           | 2658                | 14543776889         | 7.49             | 102575               |
| 9           | 15355243313       | 46.55           | 8024                | 14562027197         | 7.39             | 24278                |
| 10          | 15867396841       | 27.08           | 793                 | 14586453979         | 7.07             | 5082                 |
| 11          | 15894595624       | 28.53           | 2069                | 14588721890         | 6.95             | 1819                 |
| 12          | 15936710950       | 31.30           | 5016                | 15579178277         | 24.14            | 39917                |
| 13          | 15996493807       | 36.61           | 40031               | 15833022245         | 26.50            | 39520                |
| 14          | 16074011649       | 47.16           | 52354               | 16059703082         | 35.05            | 5406                 |
| 15          | 16160965257       | 69.73           | 20842               | 16247173522         | 42.95            | 3217                 |
| 16          | 16239011987       | 124.65          | 1201                | 16378170780         | 80.48            | 2358                 |
| 17          | 16290249709       | 264.02          | 1865                | 16239569727         | 9.44             | 7315                 |

Figure 2. FEM meshes for original (black) and optimized (red) choke-mode cavities.

4. Shape optimization of crab cavity

The second shape optimization example is the design of a crab cavity which will be a potential upgrade of the Large Hadron Collider (LHC) at CERN. The main design goal is to minimize the peak value of the magnetic field on the cavity surface, and constrain cavity frequency at 800 MHz. This is a challenging problem, since as the cavity deforms the location of the peak value can change in a non-smooth fashion so that the derivative of the objective function with respect to design parameters is not continuous. As a result, we use $L_p$ norm in the objective function. We start with small $p$ and increase this value and follow a continuation strategy. As $p$ approaches infinity, $L_p$ norm approaches to infinity norm. Numerical care must be taken to prevent overflow when $p$ is too large.
The FEM mesh and definition of design parameters are shown in Figure 3. The sum of CAD parameters $a$ and $A$ fixed, and there are 4 independent design parameters. We consider two cases, with different bounds for design variables. In the first case the bound is set to $0.01m$, and in the second to $0.03m$. Table 3 shows stages of continuation for Case 1. Optimization start with $p = 64$, and terminates when $p = 16384$. Tables 4 shows maximum magnetic field values for initial and optimum cavities for Case 1 and 2. Finally optimum design parameters are listed in Table 5. The optimization procedure succeeds in decreasing the maximum value of magnetic field considerably while constraining the operating frequency.

### Table 3. Initial and optimized magnetic $|B|_p$ and electric $|E|_p$ values with increasing $p$ values and corresponding infinity norms.

| $p$  | $|B|_p$   | $|E|_p$   | $|B|_\infty$ | $|E|_\infty$ |
|------|-----------|-----------|--------------|--------------|
| 64   | $9.975e-8$ | $28.753$  | $1.131e-7$   | $34.919$     |
|      | $9.404e-8$ | $29.417$  | $1.100e-7$   | $35.904$     |
| 256  | $1.045e-7$ | $34.068$  | $1.100e-7$   | $35.904$     |
|      | $1.012e-7$ | $33.233$  | $1.063e-7$   | $35.009$     |
| 1024 | $1.049e-7$ | $34.556$  | $1.063e-7$   | $35.009$     |
|      | $1.041e-7$ | $34.331$  | $1.054e-7$   | $34.779$     |
| 4096 | $1.050e-7$ | $34.667$  | $1.054e-7$   | $34.779$     |
|      | $1.049e-7$ | $34.656$  | $1.053e-7$   | $34.768$     |
| 16384| $1.052e-7$ | $34.740$  | $1.053e-7$   | $34.768$     |
|      | $1.051e-7$ | $34.741$  | $1.052e-7$   | $34.769$     |

### Table 4. Initial and optimum field values for Case 1 and Case 2.

|          | $|B|_\infty$ | $|E|_\infty$ |
|----------|--------------|--------------|
| Initial  | $1.131e-7$   | $34.919$     |
| Case 1   | $1.052e-7$   | $34.769$     |
| Case 2   | $1.055e-7$   | $34.858$     |


Table 5. Optimum design parameters in terms of change in CAD parameters.

|       | ∆A    | ∆a    | ∆B    | ∆b    | ∆l    |
|-------|-------|-------|-------|-------|-------|
| Case 1| -0.00307 | 0.0307 | -0.01 | 0.004105 | 0.00390 |
| Case 2| -0.00305 | 0.0305 | -0.03 | 0.004084 | 0.01991 |

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