CEFC1179

SLAC-PUB-10496
June 2004

Adaptive Mesh Refinement for High Accuracy Wall Loss Determination in Accelerating Cavity Design*

Lixin GE, Lie-Quan LEE, Zenghai LI, Cho NG and Kwok KO[1]
Yunhua LUO, Mark SHEPHARD[2]

Abstract--**This paper presents the improvement in wall loss determination when adaptive mesh refinement (AMR) methods are used with the parallel finite element eigensolver Omega3P. We show that significant reduction in the number of degrees of freedom (DOFs) as well as a faster rate of convergence can be achieved as compared with results from uniform mesh refinement in determining cavity wall loss to a desired accuracy. Test cases for which measurements are available will be examined, and comparison with uniform refinement results will be discussed.**

Index Terms--**Adaptive mesh refinement, finite element analysis, wall losses, error estimator**

I. Introduction

Wall loss calculations are becoming increasingly important in accelerator cavity design, especially for next generation high energy accelerators which plan to operate at higher currents and energies. In an accelerating cavity, increased wall loss reduces the shunt impedance and at high power, can lead to RF surface heating that degrades the cavity's performance. Determining wall loss in complex cavity shapes requires numerical modeling which becomes more difficult when external coupling is introduced into the cavity. This causes the wall currents to localize in narrow regions around the coupling iris, making accurate wall loss calculation a challenging task. As part of the DOE SciDAC Accelerator Simulation project, SLAC and RPI are collaborating on the development of an adaptive mesh refinement (AMR) capability to improve the accuracy and convergence of wall loss (or quality factor) calculations in accelerating cavities. Specifically, the effort focuses on combining the parallelism and higher-order finite element formulation of SLAC's eigensolver Omega3P and the mesh adaptation and geometry modules developed at RPI to provide a design tool that can predict a cavity's properties such as frequency and quality factor reliably and with high accuracy.

II. Adaptive Mesh Refinement (AMR)

The approach consists of interfacing SLAC's parallel eigenmode solver Omega3P to RPI-SCOREC's meshing module to form a refinement loop (Fig.1). Beginning with an initial coarse mesh, Omega3P calculates the starting field solutions from which error estimates are derived [1-2] to provide as input to the meshing module. Based on the error estimates, the initial mesh is then modified in reference to the CAD model and a new mesh is generated for the next execution of Omega3P. This iterative procedure repeats until the desired accuracy is reached.

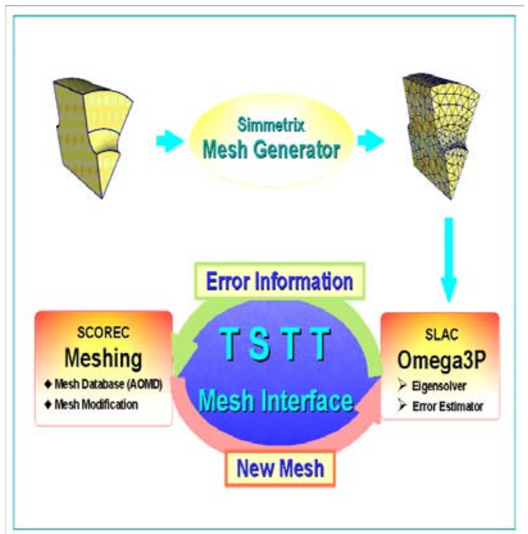

Fig. 1 SLAC-RPI AMR loop.

A. *Eigenmode Calculations*

Omega3P belongs to a suite of codes that includes time and frequency domain solvers that are based on tetrahedral mesh and finite element basis functions up to 6th order. The target applications are large, complex 3D accelerator components and beamline systems. Its development has been motivated by the need of the Next Linear Collider (NLC) project for a modeling tool that can provide frequency accuracy of 0.01%. The eigensolver incorporates the AV formulation and consists of an iterative method based on an Inexact Shift-Invert Lanczos algorithm, as well as an Exact Shift-Invert Lanczos scheme using SuperLU or WSMP as the direct linear solver. Parallelization is based on MPI and the code is portable to any Operating System in which an MPI implementation is available. The largest eigen-problem solved to date is 93 million DOFs on 1024 IBM Power3 375MHz processors, taking about 700 GB memory and 420 minutes [3] to obtain 12 eigenvalues and their corresponding eigenvectors. The code has succeeded in meeting the NLC design requirements and is being applied routinely to simulate large structures consisting

*Manuscript received January 15, 2004. This work was supported by the U.S. Department of Energy under Contract No. DE-AC03-76SF00515.

[1]Stanford Linear Accelerator Center, Stanford University, USA (telephone: 650-926-3863, e-mail: lge@slac.stanford.edu).

[2]Scientific Computation Research Center, Rensselaer Polytechnic Institute, USA.

Presented at the Eleventh Biennial IEEE Conference on Electromagnetic Field Computation, Seoul, South Korea, June 6-9, 2004

of many cavities that cannot be modeled by codes running on a single CPU.

B. Error Estimator

In AMR, the Zienkiewicz-Zhu (ZZ) method is used as the error estimator for mesh modification due to its advantages of simplicity in implementation and cost effectiveness [1-2]. From the Omega3P eigensolver, we obtain the numerical field solutions and their derivatives which are regarded as the raw field data E_{raw}, H_{raw}, ∇E_{raw} and ∇H_{raw}. In the ZZ error estimator, the basic assumption is that based on the raw fields, we can construct more accurate recovered fields E_{rec}, H_{rec}, ∇E_{rec} and ∇H_{rec}. Under this assumption, the error in the primary field or derived field is the difference between the raw field and the recovered field, which is measured by the L-2 norm

$$err = \|E_{raw} - E_{rec}\|_{L2}, \qquad err = \|H_{raw} - H_{rec}\|_{L2},$$

or

$$err = \|\nabla E_{raw} - \nabla E_{rec}\|_{L2}, \quad err = \|\nabla H_{raw} - \nabla H_{rec}\|_{L2}.$$

The parameter err is a piecewise continuous function which we integrate over each element to get an error for that element. For a given threshold, we judge which elements need to be refined or coarsened. The refine-coarsen process will be stopped if the total error δ is less than a specified value where

$$\delta = \int_{\Omega} \eta d\Omega = \sum_{i=1}^{N} \eta_i = \sum_{i=1}^{N} \int_{\Omega_i} \eta d\Omega_i$$

and δ : the sum of errors from all the elements,
Ω : the whole solution domain,
Ω_i : the i$^{\text{th}}$ element domain,
N : the total number of elements.

C. Mesh Adaptation

Based on the error field derived above, a mesh size field is generated by performing an optimization that minimizes the total number of elements in the whole domain subject to a constraint set by the local error field and size field. The mesh size field is used as the input to the mesh modification package to perform mesh refinement or coarsening and smoothing.

RPI's mesh modification package [4-6] contains a general mesh adaptation procedure that applies mesh modification operations to yield a mesh of the same quality as one that would be obtained by the standard re-meshing procedure but at less computational cost [7]. In particular, based on the 3-D geometry model and the corresponding tetrahedral mesh, the package can effectively modify the starting mesh until the target element size and shape distribution are met with the curved domain boundaries properly approximated.

III. NUMERICAL RESULTS

A. Trispal 4-Petal Accelerating Cavity

The first test case for the AMR procedure is the Trispal 4-petal accelerating cavity for which measured data are generally available [8-10]. Frequency and quality factors are known for the zero and pi modes so that direct comparison with simulation can be made to provide a benchmark for the method. The Trispal 4-petal accelerating cavity (CEA, France) is a 2 cell cavity in which the cells are coupled through 4 "petal" holes in the common cavity wall. The coupling hole influence on Q is quantified by $\Delta Q / Q$, which is defined as the factional change in Q as a result of the cell-to-cell coupling when compared with the uncoupled cavity. .

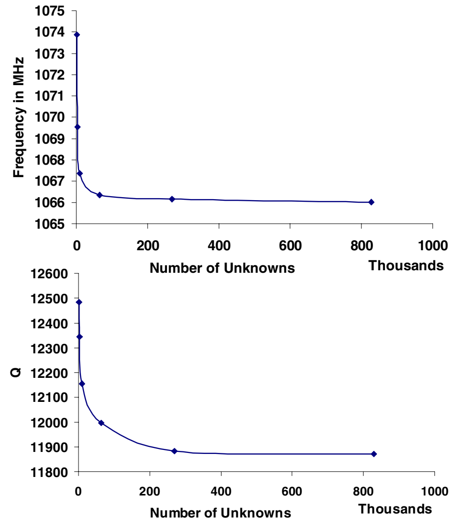

Fig. 2 Frequency (Top) and Q (Bottom) convergence vs. the number of unknowns for the pi mode in the Trispal cavity.

Fig.2 shows the convergence of frequency and Q with the number of unknowns for the pi mode where each data point represents a refinement step. Fig.3 shows the mesh and wall loss distribution on the cavity surface for three AMR steps with increasingly denser mesh in the area of high field concentration (from left to right). Table I shows the Omega3P results with AMR and with uniform mesh refinement (UMR) and how they compare with measurement data for the pi and zero modes. We can see that the AMR capability provides a much closer agreement to measured data and requires a much reduced number of DOFs, clearly demonstrating its advantage in generating the optimal mesh for accurate wall loss calculations.

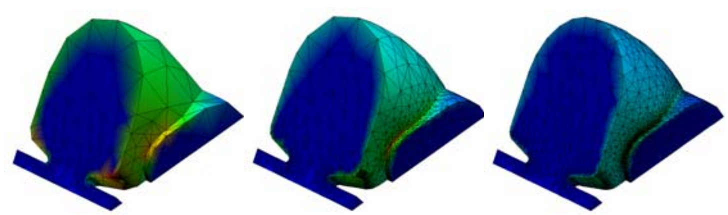

Fig. 3 Mesh and wall loss distribution for three AMR steps.

	Frequency (MHz)		Q Factor		dQ/Q	
Mode	Pi	Zero	Pi	Zero	Pi	Zero
Measurement	1064	1072	11340	12938	-22.5%	0.9%
Omega3P (UMR)	1066	1074	12111	13738	-19.6%	3.4%
Omge3P (AMR)	1066	1074	12004	13688	-21.7%	1.4%

Table I. Comparisons among measured data, Omega3P with AMR & Omega3P with UMR on Trispal 4-petal cavity.

B. NLC Damped Detuned Structure

The Damped Detuned Structure (DDS) [11-12] is the baseline linac structure design for the NLC, a proposed DOE accelerator for high energy physics research. The important requirements for the DDS cavity are that the accelerating mode frequency has to be known to within 0.01% of the designed value, and that the wall loss to be calculated as accurately as possible for efficiency and thermal management reasons. Previously, Omega3P calculations have shown capable of meeting these requirements using uniform refinement and they form the basis on which the NLC linac has been developed and prototyped. The goal of the AMR is to improve on this design procedure by reducing both manual and computing resources.

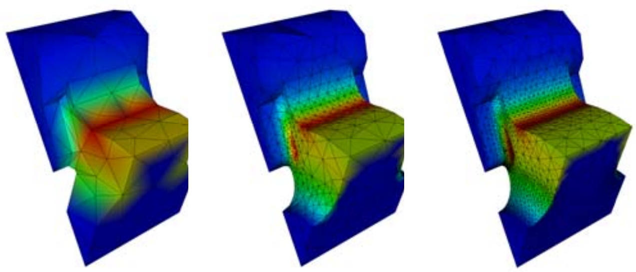

Fig. 4 Mesh and wall loss distributions corresponding to three AMR steps for the DDS pi mode from Omega3P solutions.

Fig. 4 shows the mesh adaptivity for the DDS pi mode as the AMR process progresses and the allocation of new mesh points to regions of high wall loss concentration. The effectiveness of the procedure is demonstrated in Fig. 5 which compares the convergence of freqency and Q from uniform refinement (Blue) and from adaptive refinement (Purple). The convergence is much faster using AMR which means a much reduced number of unknowns is needed to reach the target accuracy. In the case of the Q calculations, the reduction is a factor of 18, which is expected to be even more significant when large problem sizes are considered.

IV. CONCLUSION

Under the DOE SciDAC Accelerator Simulation project, SLAC and RPI are working together on the development of an adaptive mesh refinement capability to improve the accuracy and convergence of wall loss determination in accelerating cavity design. The adaptive procedure has been implemented in the parallel finite element eigensolver Omega3P and applied to the Trispal 4-petal accelerating cavity, for which measured data are available as a benchmark test. When applied to the NLC DDS cavity, an order of magnitude reduction in the number of unknowns has been achieved to obtain the desired accuracy. The team is now focused on implementing a parallel AMR capability to further reduce the amount of computing and human effort involved in these important computations that are necessary for next-generation accelerator development.

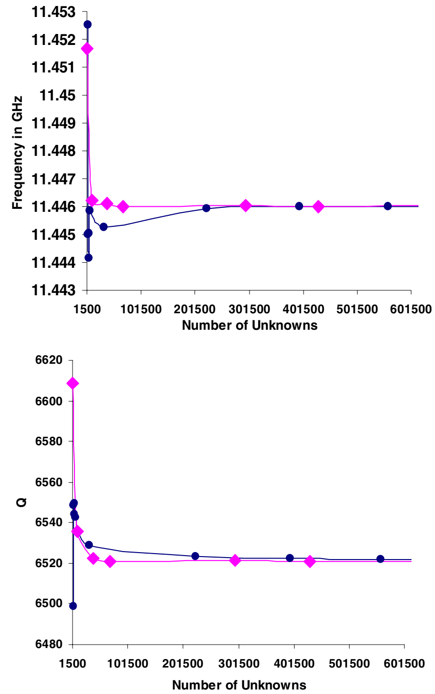

Fig. 5 Frequency (Top) and Q (Bottom) convergence vs. number of unknowns for DDS pi mode with blue line denoting uniform refinement and purple line denoting adaptive refinement.

REFERENCES

[1] O. C. Zienkiewicz, and J. Z. Zhu, "The superconvergent patch recovery and a posteriori error estimates. Part 1: The recovery technique", International Journal for Numerical Methods in Engineering, Vol. 33, pp. 1331-1363, 1992.

[2] O.C. Zienkiewicz and J. Z. Zhu, "The superconvergent patch recovery and a posteriori error estimates. Part 2: Error estimates and adaptivity", International Journal for Numerical Methods in Engineering, Vol. 33, 1365-1382, 1992.

[3] Lie-Quan Lee et al "Solving large sparse linear systems in end-to-end accelerator structure simulations", SLAC-PUB-10320, January, 2004.

[4] M. W. Beall and M. S. Shephard, "A general topology-based mesh data structure", International Journal for Numerical Methods in Engineering, 40: 1573-1596, 1997.

[5] K. E. Jansen, M. S. Shephard, and M. W. Beall, "On anisotropic mesh generation and quality control in complex flow problems", In Tenth International Meshing Roundtable, 2001.

[6] X. Li, M. S. Shephard, and M. W. Beal "Accounting for curved domains in mesh adaptation", International Journal for Numerical Methods in Engineering, 58: 247-276, 2003.

[7] Xiangrong Li, M. S. Shephard and Mark W. Beall, "3-D anisotropic mesh adaptation by mesh modification", submit to Computer Methods in Applied Mechanics and Engineering.

[8] P. Balleyguier, "Coupling slots without shunt impedance drop", Linac 96, Geneva, p. 414

[9] P. Balleyguier, "Coupling Slots Measurements Against Simulation For Trispal Accelerating Cavities", Linac 98, Chicago, p.130.

[10] P.Balleyguier et al, "Improvement in 3D Computation of RF-Losses in Resonant Cavities", XX International Linac Conference, 2000, Monterey, California, August 21-25, 2000.

[11] Z. Li, et al, "Design of the JLC/NLC RDDS structure using parallel eigensolver Omega3P", XX International Linac Conference, Monterey, California. August 21-25, 2000.

[12] Z. Li, et al, "Parameter Optimization for the Low Frequency Linacs in the NLC", PAC99, 03/29-04/02, 1999.