BENCHMARK OF DIFFERENT ELECTROMAGNETIC CODES FOR THE HIGH FREQUENCY CALCULATION*

K. Tian[#1], G. Cheng[1], F. Marhauser[1], H. Wang[1], C. D. Zhou[2]

[1]Thomas Jefferson National Accelerator Facility, Newport News, VA 23606, USA

[2]Tech-X Corp., Boulder, CO 80303, USA

Abstract

In this paper, we present benchmarking results for high-class 3D electromagnetic (EM) codes in designing RF cavities today. These codes include Omega3P [1], VORPAL [2], CST Microwave Studio [3], Ansoft HFSS [4], and ANSYS [5]. Two spherical cavities are selected as the benchmark models. We have compared not only the accuracy of resonant frequencies, but also that of surface EM fields, which are critical for superconducting RF cavities. By removing degenerated modes, we calculate all the resonant modes up to 10 GHz with similar mesh densities, so that the geometry approximation and field interpolation error related to the wavelength can be observed.

INTRODUCTION

Numerical EM simulations are very important for designing and optimizing new cavity structures, investigating the RF breakdown fields in cavity operation, and studying beam dynamics in RF cavities. The major concern of the numerical EM codes is accuracy. For the R&D of superconducting RF cavities, accuracy of the surface EM fields is particularly important for many advanced RF problems such as multipacting and Lorentz force detuning.

Several EM codes, either developed by commercial companies or nonprofit research institutes, are utilized for RF cavity related simulations. Most of these codes provide good benchmark results against a simple pillbox cavity for the accuracy of frequency and EM fields. However, a real RF cavity is usually much more complex than a pillbox structure, and normally featured with curved 3-D surface. Due to measurement errors and unpredictable operating complexity, it is often difficult to conduct a good comparison between numerical simulation results and measured data. Spherical cavities are ideal benchmarking models due to their real curved 3-D surface and the availability of analytical solutions. Thus, we can compare the integrity of results from different EM codes for same spherical cavity models.

ANALYTICAL SOLUTIONS

In this paper, we use r, θ, and φ to denote the radial distance, zenith angle, and azimuth angle in a spherical coordinate system, respectively. As shown in Fig.1, we use two different spherical models for the benchmarking:

one is a simple cavity bounded by conductor at r=a; the other model is formed by subtracting two cones from a concentric sphere (d<r<b). Throughout this paper, we will call the first cavity single sphere, and the second cavity double sphere. We have chosen a=b=10 cm and d=5 cm.
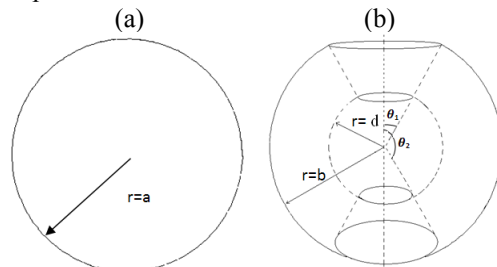

Figure1: Two spherical cavities.

The electromagnetic fields inside a spherical cavity can be obtained by solving Helmholtz equations in spherical coordinates using the Borgnis technique as shown in Ref [6]. For simplicity, we assume that the EM fields, rotationally symmetric, are independent of the azimuthal angle φ. Under this assumption, if we choose the radial direction as the longitudinal direction in a spherical cavity, the EM fields can be classified into TM and TE modes, whose general solutions of EM fields are shown in Eq. (1) and (2), respectively:

$$\begin{cases} E_\theta = \frac{1}{r}\frac{\partial^2 U}{\partial\theta\partial r} \\ E_r = \frac{\partial^2 U}{\partial^2 r} + k^2 U \quad (1) \\ H_\varphi = -\frac{j\omega\varepsilon}{r}\frac{\partial U}{\partial\theta} \end{cases} \qquad \begin{cases} E_\varphi = -\frac{j\omega\mu}{r}\frac{\partial V}{\partial\theta} \\ H_\theta = \frac{1}{r}\frac{\partial^2 V}{\partial\theta\partial r} \qquad (2) \\ H_r = \frac{\partial^2 V}{\partial^2 r} + k^2 V \end{cases}$$

where μ is the vacuum permeability; ε is the vacuum permittivity; ω is the angular frequency; U and V, the electrical and magnetic Borgnis functions [6], have different forms for these two cavities. The maximum surface electric fields of TM modes for the single sphere only occur at the two poles, which are two points. As to TE modes, the surface electric fields vanish in both models. In order to benchmark the analytical results of maximum surface electric fields against simulations, we need to solve TM modes of the double spherical cavity. For benchmarking of maximum magnetic fields, we have chosen TE modes in the single sphere due to its relatively simple analytical computation.

For TE modes of the single sphere:

$$V = B_n\sqrt{r}J_{n+\frac{1}{2}}(kr)P_n(cos\theta) \qquad (3)$$

where B_n is a constant, and k is the wave number. Substituting Eqn. (3) to (2), we can obtain the fields expressions with the only undefined parameter B_n.

Boundary conditions on the spherical surface lead to dispersion equations:

$$[\sqrt{y}J_{n+\frac{1}{2}}(y)]|_{y=ka} = 0. \qquad (4)$$

$$\omega_{TE_{nop}} = \frac{y_{np}}{a\sqrt{\mu\varepsilon}} \qquad (5)$$

where y_{np} is the pth root of Eqn. (4). On the surface of the sphere, all other field components vanish except

$$H_\theta = -\frac{B_n}{\sqrt{a}}kJ'_{n+\frac{1}{2}}(ka)P_n^1(cos\theta) \qquad (6)$$

which is only dependent on θ. In order to compare the maximum fields calculated from analytical solutions and different codes, we choose the normalized stored energy to be equal ε/2 in value. By integrating the electric fields over the whole volume, we can calculate the stored energy and thus determine the value of B_n and fields distributions. Then the maximum magnetic fields can be derived from Eqn. (6).

To solve TM modes of the double sphere cavity, we used θ_1=tan^{-1}(8/15) and θ_2=π-θ_1. The Borgnis function is:

$$U = [A\sqrt{r}J_{v+\frac{1}{2}}(kr)+B\sqrt{r}N_{v+\frac{1}{2}}(kr)][CP_v\ (cos\theta) + DP_v\ (-cos\theta)], \qquad (7)$$

where A, B, C, D are constants. For this cavity, field expressions contain both Bessel and Neumann functions, and v is not an integer any more. Field components can be derived by substituting Eqn. (7) in (1). The boundary conditions at four external surfaces are: E_r=0 at θ= θ_1 and θ_2; E_θ=0 at r=d and b. Using the similar technique as the single sphere, (9) the angular frequency of any TM_{v0p} mode can be derived from boundary conditions. We calculate the stored energy by integrating the magnetic fields and normalize its value to equal ε/2. Then, all coefficients in Eqn. (7) can be solved using boundary conditions. The maximum surface electric filed then can be determined.

All the numerical calculations, such as the integration and roots of different mathematic equations etc., were done by using MATLAB [7] with a tolerance of 1e-16.
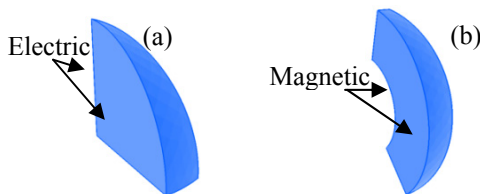
BENCHMARKING RESULTS

Figure 2: Simulation volumes for (a) single sphere; (b) double sphere

Since only azimuthally independent modes are of interest, we can simulate partial volumes with proper boundary conditions. This not only enhances the computing efficiency, but helps us to suppress the degenerated modes. As shown in Fig. 2, we simulated a sector of 18 degree azimuthally. For TE modes of the single spherical cavity, we further cut it at its equatorial symmetry plane, generating a simulated volume of 1/40 of the whole sphere. By setting two side planes as electric boundaries and alternating the symmetric plane as electric or magnetic boundary, we can solve all TE modes. For the double sphere we did not cut the 18 degree sector into half, so the simulated model is 1/20 of the whole double sphere. By setting two side planes as magnetic boundaries, we can obtain all TM modes. We have simulated modes of these two cavities up to 10 GHz using Omeg3P 7.2.1, VORPAL 4.0, CST Microwave Studio (MWS) 2009 (and 2008), HFSS 11.0, and ANSYS 11.0. Omega3P, HFSS, and ANSYS utilize Eigen solvers for EM problems based on the Finite Element Method (FEM), The Eigen solver of CST MWS uses the Finite Integration Method and meshing is done by a Perfect Boundary Approximation® method. VORPAL implements the finite-difference-time-domain integration of the EM field on a Yee mesh. Among all these codes, Omega3P, VORPAL, MWS, and ANSYS are capable of parallel computation. In the following, we summarize the simulation conditions of each code.

Omega3P: For the single sphere cavity, we ran the code with one CPU for 2 hours on a local server, having 4 CPUs and 8GB RAM memory. The double sphere was simulated on Bassi at NERSC, with rather massive parallel computing environment, in less than 30 minutes. We automatically meshed the volume with an unstructured 10-point tetrahedral mesh with a mesh size of 2mm using CUBIT [8]. The accuracy is recorded by the given residual number, typically less than 1e-7.

VORPAL: The single spherical cavity is simulated as 1/20 of the whole sphere without a cut at its equator. VORPAL time-domain simulations are split into 3 runs to cover different frequency range. The filter-diagonalization method (FDM) [9] is used to extract the frequency and construct the field pattern of each TE mode. For a 2mm uniform mesh size, each VORPAL run takes about 3 hours with 16 CPUs on a local Linux cluster. The time for FDM analysis is negligible with integrated frequency analysis tools in VORPAL VIEW. The benchmarking against the double sphere is still in progress when the paper is written.

ANSYS: Both cavities were run on a local windows server in parallel processing mode with four Intel Xeon CPUs and took about 1 hour for each cavity. A uniform 2mm tetrahedral mesh was constructed in ANSYS models.

MWS: The simulation was divided in several runs on a PC with 1 CPU and 3 GB RAM. 2mm mesh size was fixed by setting the upper frequency limit. We used the AKS solver for the lower frequency band and the JDM solver for the higher frequency band. The CPU time varied from a few minutes to 6 hours depending on the solver settings. The accuracy of each solution is checked after the calculation by using Maxwell equations.

HFSS: Same PC used as for MWS. The simulation was also split into several runs, with each run only covering 10 modes. The mesh scheme was based on a 2mm maximum mesh length for both the volume and the sphere surface. Adaptive meshing was used during the iterations. The CPU time varied from a few minutes to about 1 hour

depending on the how fast the modes converged. For sufficient accuracy, the maximum deviation in the mode frequency per simulation pass was set at 0.01%.

All relative errors in this paper are defined as:

$$Rel.Error = \left| \frac{|X_s| - |X_A|}{|X_A|} \right|, \tag{8}$$

where X_s represents the simulation result of resonant frequency or the maximum EM field on surface; X_A represents the corresponding analytical result. Fig. 3 presents results of resonant frequencies for both the single and double sphere. One should note that HFSS and MWS could not provide solutions for the double sphere for modes higher than about 6 GHz within a reasonable CPU time. The comparison indicates that solutions from Omega3P are consistently more accurate than those from other codes. Its accuracy is well below 10^{-5}. With increasing frequency, the mesh number per wavelength decreases, therefore relative errors for most codes increase as expected. An interesting exception is that relative errors achieved with ANSYS kept rather constant at about $2x10^{-5}$.
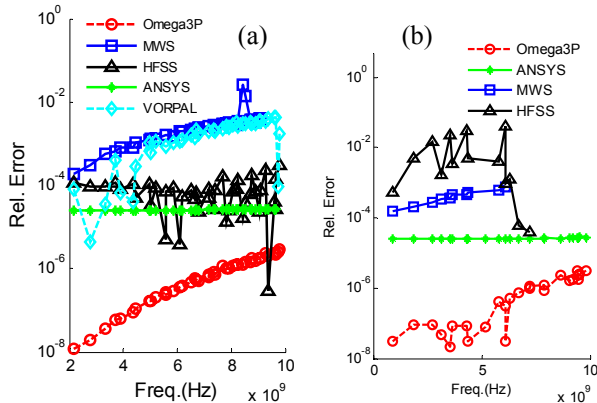

Figure 3: Relative errors of frequencies achieved with various codes for (a) single sphere and (b) double sphere.

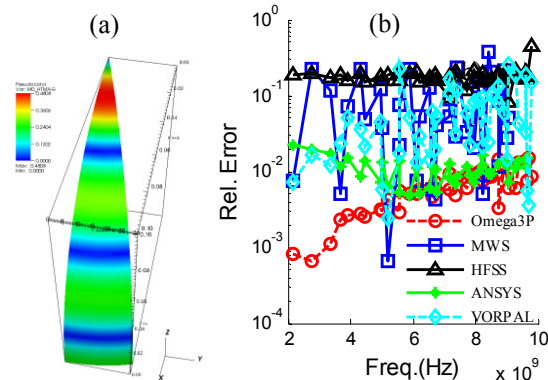Figure 4: (a) An example of strap-like surface magnetic field; (b) relative errors of the maximum surface (r =10cm) magnetic fields of the single sphere.

To exclude non physical (poor accuracy) or degenerated modes from simulations, the rule of thumb is to choose only those modes with strap-like pattern of the amplitude surface EM fields (Fig. 4(a)). Relative errors for surface EM fields are plotted in Fig. 4(b) and Fig. 5. Omega3P has overall yields the best accuracy, ranging

from 10^{-4} to 10^{-2} for the magnetic fields and from 10^{-5} to 10^{-2} for the electric fields. Results of ANSYS are not consistent, better for the single sphere, and on the inner surface of the double sphere, but not as good on its outer surface. VORPAL is still comparable with MWS, but HFSS shows very poor accuracy for all cases.
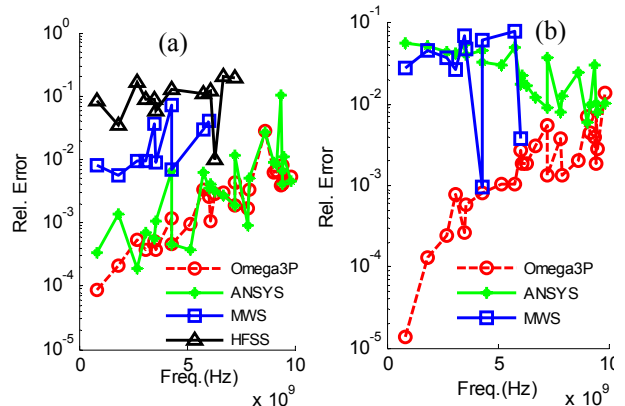

Figure 5: Relative errors of the maximum surface electric fields for the double sphere. (a) Inner surface; (b) outer surface.

CONCLUSIONS

The accuracy of a numerical simulation is affected by many factors, such as the meshing, algorithms, EM solver types, and interpolation techniques etc. In addition, each different code has its own unique advantages and disadvantages. The benchmarking results in this paper do not intend to favor a specific code to another. However, by choosing a unique analytical model, common simulation settings for all different codes, and most importantly, the same cavity geometry, the results provide better understanding of the performance and limitations of different EM codes, especially when calculating surface fields, which are of high importance for many cavity related phenomena.

ACKNOLWGEMENT

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