BENCHMARKING DIFFERENT CODES FOR THE HIGH FREQUENCY RF CALCULATION*

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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 of cavity operation, and studying beam dynamics in RF cavities. Hence, it is very important to understand the accuracy, limitation, and capability of an EM code before applying an EM code in analyzing such problems. For many advanced problems in superconducting RF cavities, high accuracy is not only demanded for the calculation of resonant frequencies but also for the surface electromagnetic fields. For example, multipacting is still an important factor that limits the performance of a superconducting cavity. To correctly predict the process of multipacting in a cavity, the second emission yields of each impact, which is dependent on the impact energy, has to be calculated accurately. Therefore, an accurate calculation of the surface EM fields is a natural requirement for simulating the multipacting process. Another example is the Lorentz force detuning [6] resulting from the interaction of the rf magnetic field with the rf wall current in superconducting cavities. Because the superconducting cavity wall is relatively thin, at high accelerating fields, the cavity shape could be significantly deformed by the inward radiation pressure on the iris wall and the outward radiation pressure on the equator. It hence is a simulation challenge to simulate the frequency shift due to this effect. Since the radiation pressure is directly calculated from the surface EM fields, the key for an accurate simulation relies on the correct prediction of the surface EM fields.

Several EM codes, either developed by commercial companies or non profit research institutes, are utilized for simulations related to RF cavities. Most of these codes provide good benchmarking 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 the pillbox structure, and normally featured with curved 3-D surface. On the other hand, due to measurement errors and unpredictable operating complexity, it is often difficult to conduct benchmarking comparison between different simulation codes using measured experimental data. In a word, the ideal benchmarking model should have 3-D curved boundaries and can be solved analytically. Spherical cavities are such candidates for the benchmarking study. In this paper, we compare the integrity of results from different EM codes using 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 the perfect conductor at r=a; the other model is formed by subtracting two cones from a concentric sphere (d<r<b). For convenience, throughout this paper, we call the first cavity single sphere, and the second cavity double sphere. We have chosen a=b=10 cm and d=5 cm.

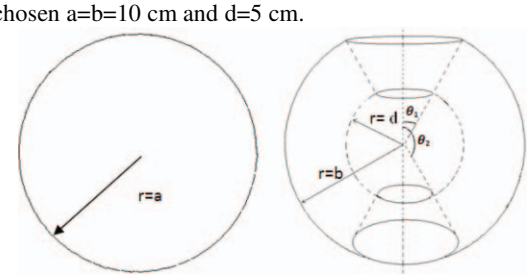

Figure1: Two spherical cavities.

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 [7]. 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 Equations. (1) and (2), respectively:

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

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

where μ is the vacuum permeability; ε is the electric permittivity; ω is the angular frequency; U and V, the electrical and magnetic Borgnis functions [7], have different forms for these two cavities.

After analyzing the analytical solutions of both single sphere and double sphere, we found out the following facts. The maximum surface electric fields of TM modes for the single sphere only occur at the two poles, which are two points. We characterize the numerical accuracy of the surface EM fields by comparing the peak values on the surface. Therefore, in order to avoid the singularity in numerical simulation, we have chosen not to use the TM modes of the single sphere for benchmarking surface electric fields. As to TE modes, the surface electric fields vanish in both models. Hence, 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. In the following, we will solve these two families of modes of our benchmarking interest.

TE modes of the single sphere

According to the Borgnis technique, in this case, U=0 and:

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

where B_n is a constant, and k is the wave number. Substituting Eq. (3) to (2), we can obtain the fields expressions with the only undefined parameter B_n. The metal boundary condition on the spherical surface leads to Eq. (4):

$$V|_{r=a} = 0 \quad (4)$$

,which can be transformed to the dispersion equation:

$$\sqrt{y} J_{n+1/2}(y)|_{y=ka} = 0 \quad (5)$$

By solving Eq. (5), we can obtain the resonant frequencies of the mode TE_{n0p}:

$$\omega_{n0p} = \frac{y_{np}}{a\sqrt{\mu_0\varepsilon_0}} \quad (6)$$

where y_{np} is the p^{th} root of Eq. (5).

For TE modes, the only component of electric filed is E_φ:

$$E_\varphi = -\frac{j\omega\mu_0 B_n}{\sqrt{r}} J_{n+1/2}(kr)\frac{dP_n(\cos\theta)}{d\theta} \quad (7)$$

so the stored energy of the whole cavity can be calculated by integrating E_φ throughout the whole spherical volume:

$$W = \frac{1}{2}\varepsilon_0 \int |E_\varphi|^2 dv \quad (8)$$

On the surface of the sphere, all other field components vanish except

$$H_\theta|_{r=a} = -\frac{B_n}{\sqrt{a}} k J'_{n+1/2}(ka) P_n^1(\cos\theta) \quad (9)$$

which is only dependent on θ.

For the purpose of benchmarking, we define the normalized surface magnetic filed as

$$h = \frac{H_\theta|_{r=a}}{\sqrt{W}} \quad (10)$$

By substituting Eqs (7)-(9) to the above expression:

$$h = \sqrt{\frac{2}{a\mu_0}} \frac{J'_{n+1/2}(ka)}{\sqrt{\int \frac{1}{r}[J_{n+1/2}(kr)\frac{dP_n(\cos\theta)}{d\theta}]^2 dv}} P_n^1(\cos\theta) \quad (11)$$

Using numerical techniques implanted in MATLAB [8], the maximum values of h for different modes can be determined. The computing precision of MATLAB is 10^{-16}, which is enough for benchmarking. We list the solutions for the first 10 modes in Table 1.

Table 1: The first 10 TE_{n0p} modes

Frequency (Hz)	n	p	h_{max}(A/m/J$^{1/2}$)
2.1439607465E+09	1	1	-19492.383
2.7499453139E+09	2	1	-21793.147
3.3341835523E+09	3	1	-25108.575
3.6859842956E+09	1	2	19492.383
3.9041824976E+09	4	1	-28186.443
4.3395438284E+09	2	2	21793.147
4.4639808826E+09	5	1	-31009.186
4.9703668154E+09	3	2	25108.575
5.0160366334E+09	6	1	-33617.568
5.2027328095E+09	1	3	-19492.383

TM modes of the double sphere

To solve TM modes of the double sphere cavity, we arbitrarily choose $\theta_1=\tan^{-1}(8/15)$ and $\theta_2=\pi-\theta_1$. The Borgnis function V=0, and

$$U = [A\sqrt{r}J_{\nu+1/2}(kr) + B\sqrt{r}N_{\nu+1/2}(kr)][CP_{\nu}(\cos\theta) + DP_{\nu}(-\cos\theta)] \quad (12)$$

where A, B, C, D are constants. For this cavity, field expressions contain both Bessel and Neumann functions, and ν 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, these conditions lead to the following two equations:

$$U|_{\theta=\theta_1,\theta_2} = 0 \quad (13)$$

$$\frac{\partial U}{\partial r}|_{r=b,d} = 0 \quad (14)$$

The condition of the existence of non zero A, B, C, and D to satisfy Eq () leads to the two eigen equations:

$$P_{\nu}(\cos\theta_1)P_{\nu}(-\cos\theta_2) - P_{\nu}(-\cos\theta_1)P_{\nu}(\cos\theta_2) = 0 \quad (15)$$

$$[\frac{1}{2\sqrt{a}}J_{\nu+1/2}(ka) + k\sqrt{a}J'_{\nu+1/2}(ka)][\frac{1}{2\sqrt{b}}N_{\nu+1/2}(kb) + k\sqrt{b}N'_{\nu+1/2}(kb)] = [\frac{1}{2\sqrt{b}}J_{\nu+1/2}(kb) + k\sqrt{b}J'_{\nu+1/2}(kb)][\frac{1}{2\sqrt{a}}N_{\nu+1/2}(ka) + k\sqrt{a}N'_{\nu+1/2}(ka)] \quad (16)$$

For a given v, the only variable in this equation is k, which is the wave number. Hence, we can obtain the resonant frequency of any TM_{v0p} mode by solving Eq. (16).

Furthermore, we define the normalized surface electric field on the two spherical surfaces as:

$$e_1 = \frac{E_r|_{r=b}}{\sqrt{W}} \quad (17)$$

and

$$e_2 = \frac{E_r|_{r=d}}{\sqrt{W}} \quad (18)$$

Table 2: The frequency and normalized maximum surface magnetic filed of the first 6 TE_{n0p} modes

Frequency (Hz)	e_{1max}(V/m/J$^{1/2}$)	e_{2max}(V/m/J$^{1/2}$)
8.377783223E+08	-22032489	-6016071
1.832902930E+09	19975209	7675141
2.713403917E+09	15231237	9805581
3.123146964E+09	8868395	-2162046
3.518547956E+09	10047403	11835720
3.598480132E+09	19323910	-4314285

Using the similar technique as the single sphere, the maximum values of e_1 and e_2 can be derived after some algebra. Results calculated from analytical solutions using MATLAB for the first six modes are listed in Table 2.

BENCHMARK RESULTS

Since only azimuthally uniform modes are of interest, we can simulate partial volumes with proper configuration of boundary conditions. This not only improves 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 both cavities. For TE modes of the single sphere, 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 equatorial 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.

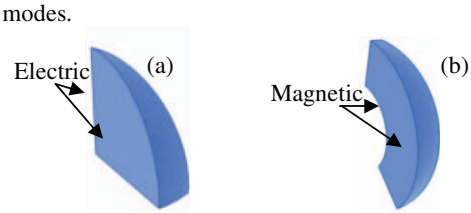

Figure 2: Simulation volumes for (a) single sphere; (b) double sphere

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

We automatically meshed both cavities with unstructured 10-point tetrahedral meshes with a mesh size of 2mm using CUBIT [9]. For the single sphere cavity, we ran the code with one CPU for 2 hours on a local server. The double sphere was simulated on Bassi at NERSC, with rather massive parallel computing environment, in about 20 minutes with 56 CPUs. The accuracy is recorded by the given residual number, typically less than 1e-7.

VORPAL

The single sphere 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) [10] 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.

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. The average mesh size of 2mm 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

The simulation was also split into several runs, with each run only covering 10 modes. The mesh scheme was based on a 2 mm average 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 converging speed of different modes. For sufficient accuracy, the maximum deviation in the mode frequency per simulation pass was set at 0.01%.

(a) (b)

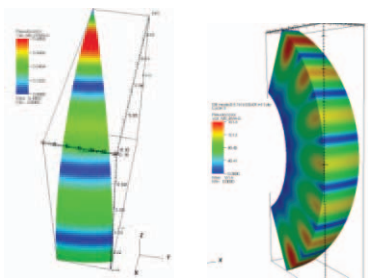

Figure 3: Examples of strap-like surface magnetic fields: (a) single sphere; (b) double sphere.

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 for the amplitude of surface EM fields. Fig. 3 shows the magnetic field distribution of a desired TM mode of the single sphere. For each mode from different simulation codes, we checked their field distribution and selected only those meeting our criteria for benchmarking.

To quantify the accuracy of simulation results, we define relative errors as the following:

$$Rel.Error = \left|\frac{|X_S|-|X_A|}{|X_A|}\right| \qquad (19)$$

where X_S can represent the simulation result of resonant frequency or the maximum EM field on surface; X_A represents the corresponding analytical result. Fig. 4 presents results of resonant frequencies for both the single and double sphere. For the double sphere, HFSS could not provide solutions 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 2×10^{-5}.

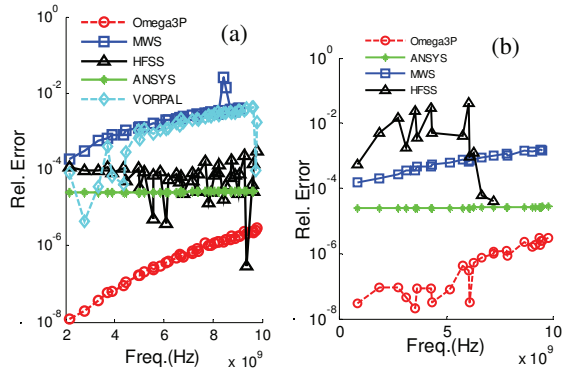

Figure 4: Relative errors of resonant frequencies achieved with various codes for (a) single sphere and (b) double sphere.

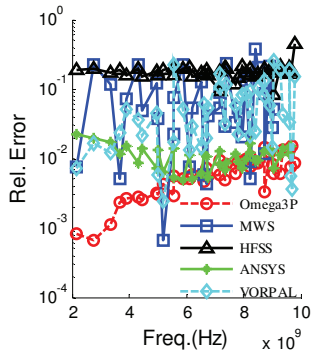

Figure 5: Relative errors of the maximum surface (r =10cm) magnetic fields of the single sphere.

Relative errors for surface EM fields are plotted in Fig. 5 and Fig. 6. Omega3P has overall 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.

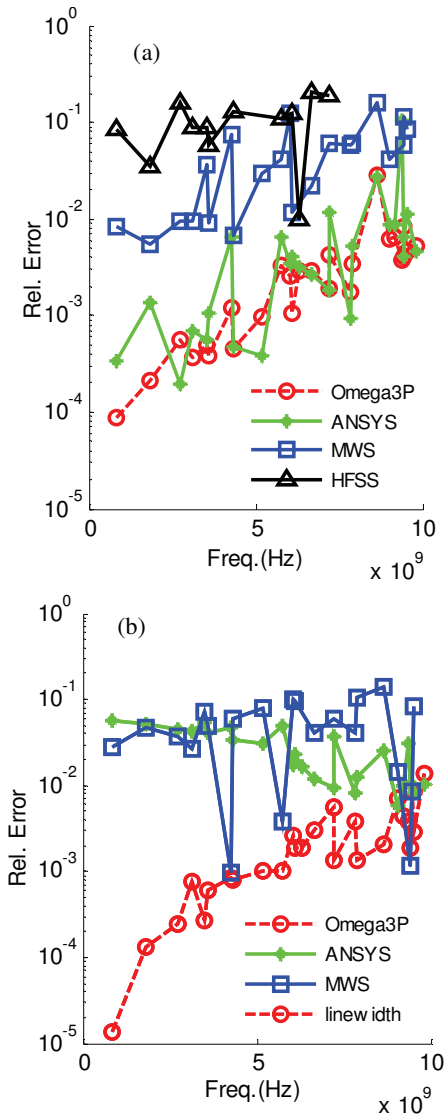

Figure 6: Relative errors of the maximum surface electric fields for the double sphere. (a) Inner surface; (b) outer surface.

CONCLUSION

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.

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