# HIGHLY ACCURATE FREQUENCY CALCULATIONS OF CRAB CAVITIES USING THE VORPAL COMPUTATIONAL FRAMEWORK[*]

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## Abstract

We have applied the Werner-Cary method [J. Comp. Phys. 227, 5200-5214 (2008)] for extracting modes and mode frequencies from time-domain simulations of crab cavities, as are needed for the ILC and the beam delivery system of the LHC. This method for frequency extraction relies on a small number of simulations, and post-processing using the SVD algorithm with Tikhonov regularization. The time-domain simulations were carried out using the VORPAL computational framework, which is based on the eminently scalable finite-difference time-domain algorithm.

A validation study was performed on an aluminum model of the 3.9 GHz RF separators built originally at Fermi National Accelerator Laboratory in the US. Comparisons with measurements of the A15 cavity show that this method can provide accuracy to within 0.01% of experimental results after accounting for manufacturing imperfections. To capture the near degeneracies two simulations, requiring in total a few hours on 600 processors were employed. This method has applications across many areas including obtaining MHD spectra from time-domain simulations.

## INTRODUCTION

Accelerator cavities are essential to such high-energy physics experiments as the Large Hadron Collider and the International Linear Collider, in addition to numerous other smaller experiments in the high-energy and medical physics fields. They are tunable devices with performance dependent on features like shape, curvature, and size.

However, it is a non-trivial task to determine the dependency of such features on cavity performance. In addition, usage of such expensive metals like niobium means design errors can be particularly costly. Coupled with the knowledge that machining can never deliver exact specifications, it is crucial to perform computational studies to understand final cavity design so as to avoid costly design errors.

Finite element simulations are presently used to compute modes of accelerator cavities within the US Department of Energy's science program [1]. Recently, a novel approach that uses the Finite-Difference Time-Domain (FDTD) method applied to Maxwell's equations for computation of frequencies and modes of accelerator cavities was reported [2]. The common approach to using the FDTD method applied to Maxwell's equations for frequency extraction is to use narrowly-filtered states combined with post-simulation FFTs. The limitations of this approach are it cannot account for degenerate frequencies and it cannot reconstruct spatial mode patterns. The new method presented by Werner and Cary in [2] overcomes these limitations.

We present work on using the Werner-Cary frequency extraction method for an aluminum model of the 3.9 GHz separators fabricated at Fermilab in 1999 for the development of a separated $K^+$ beam. Previously, experimental frequency measurements obtained from bead pull experiments were reported in [3], in addition to computational frequency measurements obtained using a finite integration method. We show here that calculations using the VORPAL computational framework along with the Werner-Cary frequency extraction method permitted discovery of machining errors that previously were not reported.

## BROADLY-FILTERED FDM

### Frequency Filtering

The first step in using FDTD simulations for frequency extraction is to create filtered states that can be used within the *Filter Diagonalization Method* (FDM). To describe the method of constructing filtered states, we present Maxwell's equations as

$$
\begin{aligned}
\frac{\partial \mathbf{B}(x,y,z,t)}{\partial t} &= -\nabla \times \mathbf{E}(x,y,z,t) \\
\frac{\partial \mathbf{E}(x,y,z,t)}{\partial t} &= -\nabla \times \mathbf{B}(x,y,z,t) - \mathbf{J}(x,y,z,t)
\end{aligned}
\tag{1}
$$

which for FDTD simulations are discretized on a regular Yee mesh [4] with electric fields placed on edges and magnetic fields located on faces as depicted in Fig. 1. The accelerator cavity is embedded within this Yee mesh and the Dey-Mittra embedded boundary algorithm [5] is used to model the curved boundaries to second-order accuracy.

The construction of filtered states is possible with an appropriately-defined current vector, $\mathbf{J}$. Putting

$$
g(t;\omega_1,\omega_2,T) = 2\left[ \frac{\sin(\omega_1(t-T/2))}{t-T/2} - \frac{\sin(\omega_2(t-T/2))}{t-T/2} \right]
\tag{2}
$$
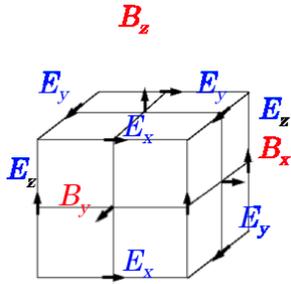
Figure 1: Electric fields on a Yee cell are placed on edges and magnetic fields are placed on faces ensuring accurate divergence calculations.

and

$$f(t) = \begin{cases} g(t; \omega_1, \omega_2, T) \exp^{-\sigma_\omega^2 (t-T/2)^2/2} & 0 \leq t \leq T, \\ 0. & \text{otherwise,} \end{cases}$$
(3)

we introduce $\mathbf{J}(x, y, z, t) = f(t)\hat{\mathbf{J}}(x, y, z)$ as a current that excites modes within the frequency range $[\omega_1, \omega_2]$. The field $\hat{\mathbf{J}}(x, y, z)$ is a spatial pattern that permits extraction of the modes of interest. See [2] for further details.

*Filter Diagonalization*

For the FDM, we use the fact that we have a field of interest, $\mathbf{s}$, which is either the electric field, $\mathbf{E}$, or the magnetic field, $\mathbf{B}$, and we have the second-order Maxwell's equation given by

$$-\frac{\partial^2}{\partial t^2}\mathbf{E}(x, y, z, t) = \nabla \times \nabla \times \mathbf{E}(x, y, z, t) = H\mathbf{E}(x, y, z, t).$$
(4)

We solve the spatial eigenvalue problem for $\nabla \times \nabla \times$ as a time evolution eigenvalue problem for $H = -\frac{\partial^2}{\partial t^2}$.

In brief, we transform the matrix $H$ by partially diagonalizing it into a block diagonal form. One large block (the filtered part) is ignored and what remains is a small block that is diagonalized by standard linear algebra routines for small matrices. Using SVD techniques, this diagonalization can be completed in a few seconds. Most of the work is getting $H$ into block diagonal form. The method can be summarized as follows:

1. Find $L$ filtered state vectors $\mathbf{s}_\ell$ that span the subspace of desired eigenmodes of $H$. $L$ must be at least as large as the number of modes in the subspace.

2. Apply $H$ to each filtered state vector to get $\mathbf{r}_\ell = H\mathbf{s}_\ell$.

3. Construct the $P \times L$ matrix $S_{p\ell} = s_{\ell,p}$ from $P$ different components of each filtered state $\mathbf{s}_\ell$, where $P \geq L$. Similarly construct $R_{p\ell} = r_{\ell,p}$.

4. Solve the generalized eigenvalue equation $S^\dagger R\mathbf{a} = \lambda S^\dagger S\mathbf{a}$ for eigenvalues $\lambda$ and eigenvectors $\mathbf{a}$. This

can be numerically challenging, so we suggest finding the eigenvalues of $S^\dagger S$ and then solving $(S^\dagger S + \alpha_{\text{cutoff}}^2)^{-1} S^\dagger R\mathbf{a} = \lambda\mathbf{a}$, where $\alpha^2$ is less than the significant eigenvalues and greater than the insignificant eigenvalues of $S^\dagger S$.

5. Eigenvalues of $H$ are the $\lambda_m$. Eigenvectors of $H$ are $\mathbf{v}_m = \sum_{\ell=1}^{L} a_{m,\ell}\mathbf{s}_\ell$.

6. If $P > L$, estimate the relative error $\epsilon_m$ of each mode (see [2]). Modes with errors near one are doubtful; if $H$ has only real eigenvalues, then modes with eigenvalues that have imaginary parts larger than the error are also doubtful. Increasing $\alpha_{\text{cutoff}}$ may vanquish doubtful modes.

## COMPUTATIONAL RESULTS

*Initial Calculations*

The FDM method applied within the VORPAL computational framework was used to extract frequencies of the A15 cavity, which is illustrated in Fig. 2. Using bead pull experiments the frequency of the $\pi$-mode was experimentally determined to be 3902.810 MHz once atmospheric factors such as humidity and temperature were taken into account [3].
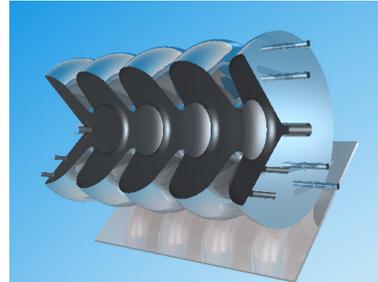


Figure 2: A15 cavity: Stack of four unpolarized dumbbells fabricated in 1999 at Fermilab for the development of a separated $K^+$ beam.

In [3], it was also noted that computer simulations used for frequency extraction yielded an error of approximately 5 MHz for the $\pi$-mode. Initial VORPAL calculations reported that the $\pi$-mode frequency was 3900.33 MHz, yielding an error of approximately 2 MHz. Convergence of the $\pi$-mode using the FDM method with VORPAL has been illustrated in Fig. 4 which also shows the Richardson extrapolation value and the experimentally-measured value.

Besides extracting frequency values, we can also reconstruct the spatial mode pattern using the FDM method with VORPAL. VORPAL uses a visualization schema (called vizschema [6]) that permits viewing of the modes with VisIt [7]. In Fig. 3 we have displayed the $z$-component of the magnetic field for the $\pi$-mode showing the correct behavior.
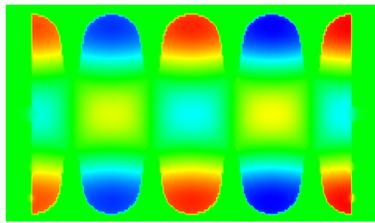
Figure 3: A slice of the $z$-component of the magnetic field for the A15 cavity's $\pi$-mode.
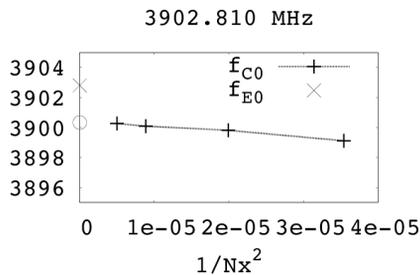


Figure 4: Convergence for the $\pi$-mode frequency for the A15 cavity. The open circle displayed on the ordinate is the value found by Richardson's extrapolation while the $\times$ on the ordinate is the experimentally determined frequency.

*Resolving Discrepancies*

Accounting for the 2 MHz difference between experimental measurements and calculations required a considerable amount of effort. A variety of sources were investigated including missing physical effects, inaccuracies in calculations, and errors in linear algebra routines. After much searching, we narrowed the discrepancy down to machining error.

In [8], the authors had noted that for a similar cavity the sensitivity of frequency with respect to equatorial radius was found to be -80.6 MHz/mm while the sensitivities of iris radius and cell half length were only -25.8 MHz/mm and 17.4 MHz/mm, respectively. Knowing that machining accuracies are 1 mil or 0.0254 mm, it seemed possible that the 2 MHz shift in the frequency of the $\pi$-mode could be the result of a 1 mil error in the equatorial radius.

Thus, we performed another set of calculations after reducing the equatorial radius by 1 mil and found the frequency of the $\pi$-mode to be 3902.5 MHz, only off by 310 kHz. See convergence plots in Fig. 5. More rigorous studies have also been performed, which will be reported in later work, that show our calculations are within measurement uncertainties.

## FINAL REMARKS

Using the VORPAL computational framework with the Werner-Cary Filter Diagonalization method, we predicted errors in machining for a stack of four unpolarized dumb-
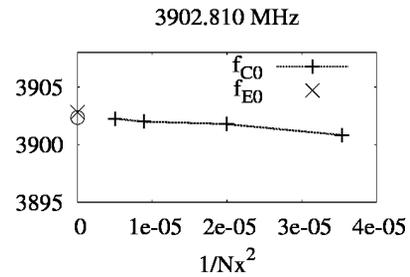


Figure 5: Convergence for the $\pi$-mode frequency for the A15 cavity with an equatorial radius smaller by 1 mil. The open circle displayed on the ordinate is the value found by Richardson's extrapolation while the $\times$ on the ordinate is the experimentally determined frequency.

bells fabricated in 1999 at Fermilab. Previously, computational errors of up to 5 MHz were reported. New results have shown that we can accurately determine frequencies to several parts in $10^5$ and thus predict that errors in machining exist. These simulations were performed on large supercomputers using up to 600 processors and delivering remarkable scalability.

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