High-accuracy Computations of RF Cavity Modes

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Outline

- Methodology
  - Assumptions
  - Algorithm
  - Embedded boundaries
  - Parallel computations
  - Richardson extrapolation
- Results for mode frequencies
  - Calculations for Crab cavities

Assumptions

Consider a system that has the form of

$$\frac{\partial^2 \mathbf{s}(t)}{\partial t^2} + H\mathbf{s}(t) = \mathbf{g}(t) \equiv f(t)\mathbf{g},$$

where $\mathbf{s}(t)$ is a state vector that evolves in time from a given initial condition, H is the discretized "$\nabla \times \nabla \times$" operator, and all the components of the driver $\mathbf{g}(t)$ have the same time–dependence $f(t)$. Let $\mathbf{v}_m$ be eigenmodes of H with

$$H\mathbf{v}_m = \lambda_m \mathbf{v}_m = k_m^2 \mathbf{v}_m$$

and we expect the solution to be the sum of oscillating eigenmodes

$$\mathbf{s}(t) = \sum_m \mathbf{v}_m [\alpha_m e^{ik_m t} + \beta_m e^{-ik_m t}],$$

where each eigenmode $\mathbf{v}_m$ oscillates at frequency $\omega_m = k_m$. The amplitudes α_m and β_m will be determined by the driver; a driver containing frequency ω such as $f(t) = \sin(\omega t)$ will excite only modes with $k_m^2 = \omega^2$. The excitation of mode m will be proportional to $\tilde{f}(k_m)$, where $\tilde{f}(\omega)$ is the Fourier transform of $f(t)$:

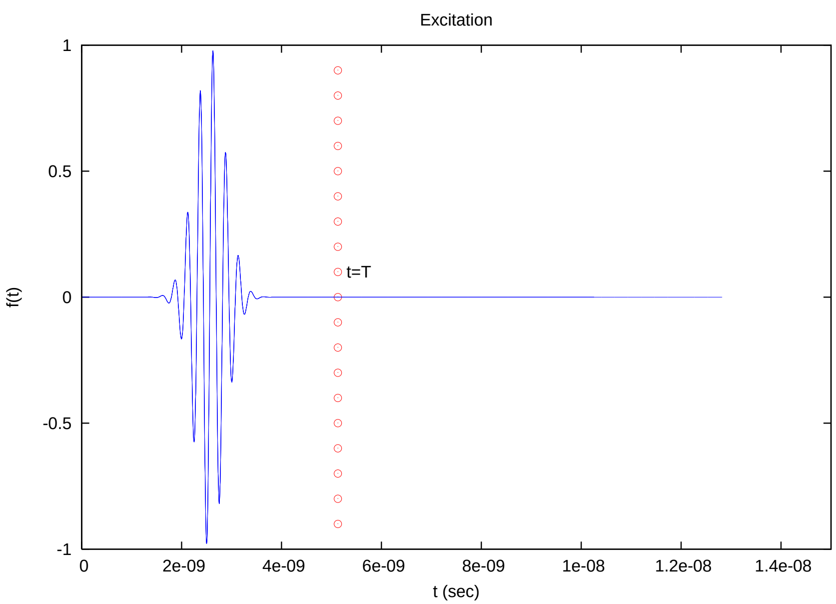
$$\alpha_m \propto \tilde{f}(k_m), \qquad \beta_m \propto \tilde{f}(-k_m).$$

Isolating a Single Mode

For simulations we need to use $f(t)$ that vanishes for $t < 0$ and $t > T$, where T is the simulation duration. For example, we employ a Gaussian-modulated sinusoid for a narrow excitation around frequency ω:

$$f(t) \propto exp[-\frac{\sigma_\omega^2 (t - t_0)^2}{2}] \sin(\omega t),$$

where $t_0 = T/2$, $t_\sigma = t_0/8.5$ and $\sigma_\omega = 1/t_\sigma$.



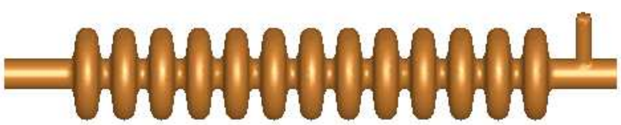
In our simulations we have:

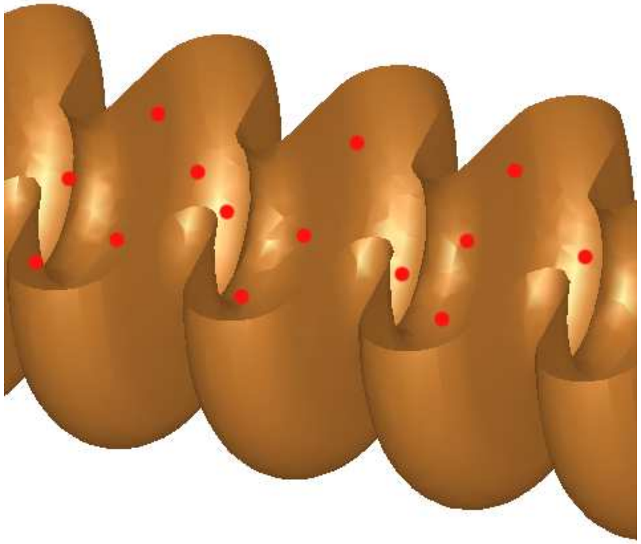
$$\nu = 3.9 \text{ GHz}, \quad \omega = 2\pi/\nu, \quad T = 20/\nu,$$

$10 - 40$ cycles of data collection.

Obtaining State Vectors

To distinguish different eigenmodes within the isolated group of M eigenmodes, one must find L state vectors such that $L \geq M$. We can find these L state vectors by running L different simulations, each excited by the same $f(t)$, but with different $\mathbf{g}$. For numerical calculations we work with just P components of the state vector $\mathbf{s_l}$. For example, we use the $p = 1, \cdots, P$ components of the vector $\mathbf{s_l}$ which we label $s_{l,p}$. In an electromagnetic simulation these components might represent the value of the electric field in state vector l at different points p, red dots in the right figure.





The Algorithm

The calculation begins with the construction of the $P \times L$ matrix S from the P components of the known vector $\mathbf{s}_l$ and matrix R from the known $\mathbf{r}_l \equiv H\mathbf{s}_l$:

$$S_{pl} \equiv \mathbf{s}_{l,p}, \qquad R_{pl} \equiv \mathbf{r}_{l,p} \ .$$

In the calculations the $H\mathbf{s}(t)$ products are approximated via

$$H\mathbf{s}(t) = -\frac{\mathbf{s}(t+\Delta t) - 2\mathbf{s}(t) + \mathbf{s}(t-\Delta t)}{\Delta t^2}.$$

Having $\mathbf{S} \equiv \mathbf{S}_{pl}$ and $\mathbf{R} \equiv \mathbf{R}_{pl}$ matrices, we first find an SVD decomposition of matrix $\mathbf{S}^T\mathbf{S}$ such that $\mathbf{S}^T\mathbf{S} = \mathbf{U}\mathbf{D}\mathbf{V}^T$, where $\mathbf{D}$ is the diagonal matrix and $\mathbf{U}$, $\mathbf{V}$ are unitary matrices. Then we find eigenvalues λ of

$$\mathbf{U}^T\mathbf{S}^T\mathbf{R}\mathbf{V}\mathbf{D}^{-1},$$

where $\tilde{D}_{kk}$ elements of $\mathbf{D}^{-1}$ are computed from D_{kk} elements of $\mathbf{D}$ via

$$\tilde{D}_{kk} = \begin{cases} 1.0/D_{kk}, & D_{kk}/D_{max} > \epsilon, \\ 0, & D_{kk}/D_{max} \leq \epsilon, \end{cases}$$

for some small ϵ. The frequencies are found as $\sqrt{\lambda}/(2\pi)$.

Conformal Boundaries, Parallel Computations and Richardson Extrapolation

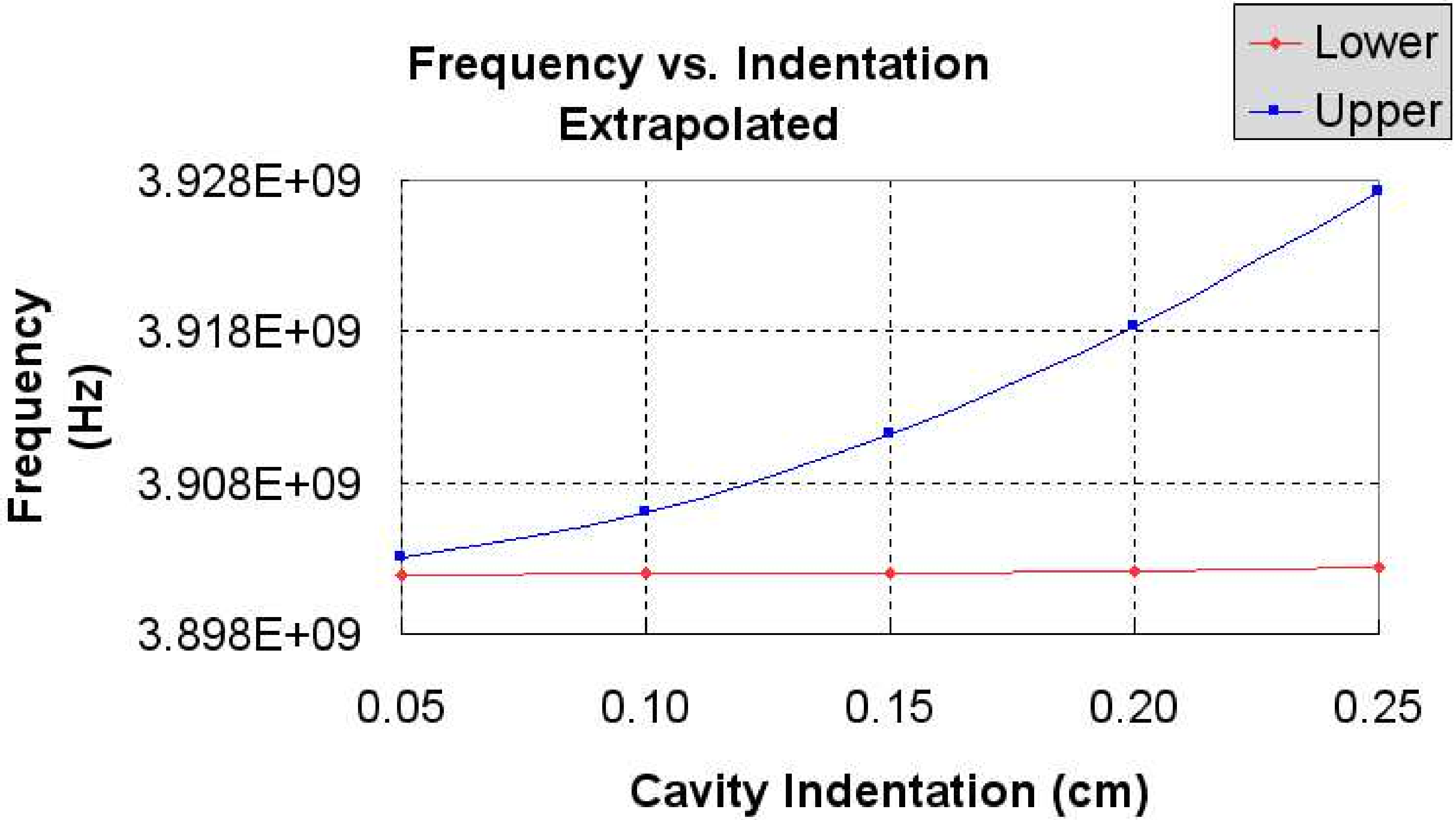
- **Conformal boundaries give second-order error in frequency** (J.R. Cary, D. Abell, J. Amundson, D.L. Bruhwiler, R. Busby, J.A. Carlsson, D.A. Dimitrov, E. Kashdan, P. Messmer, C. Nieter, D.N. Smithe, P. Spentzouris, P. Stoltz, R.M. Trines, H. Wang, G.R. Werner, Petascale Self-consistent Electromagnetic Computations Using Scalable and Accurate Algorithms for Complex Structures, Journal of Physics: Conference Series, 46 (2006) 200-204)) – **VORPAL** using FDTD approach

- **High resolution achieved through parallel computation**: 10^7 cells are needed to achieve one part in 10^5 accuracy – **VORPAL**

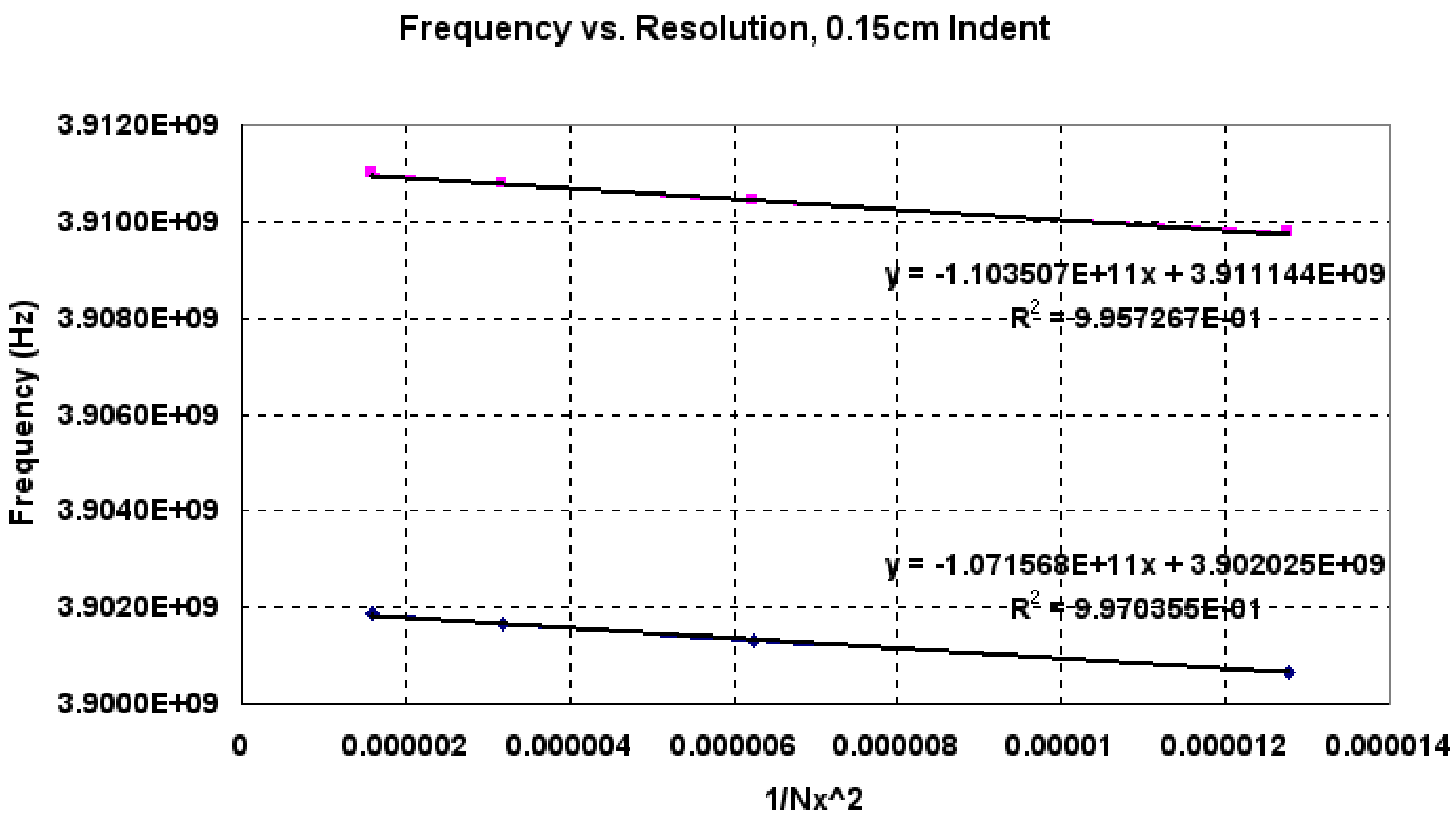
- **Frequency extraction for nearly degenerate modes obtained from Werner-Cary subspace diagonalization** (G.R. Werner and J.R. Cary, Extracting Degenerate Modes and Frequencies from Time Domain Simulations, J. Comp. Phys., submitted (2007)) – post-processing

- **Richardson extrapolation moves error to third order** – post-processing

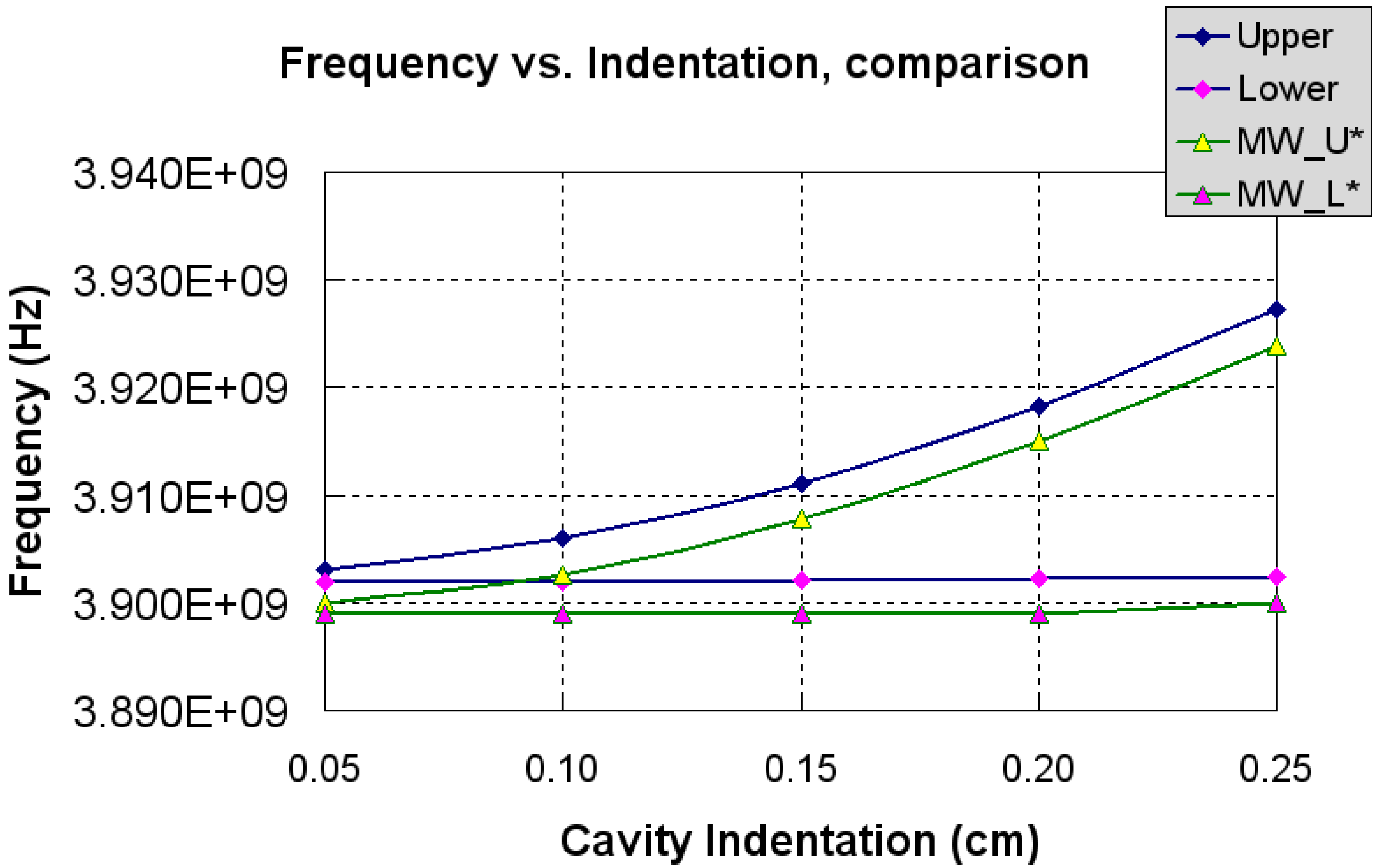
9-Cell Crab Cavity: Frequency Separation



Richardson Extrapolation



Comparison



[G.C. Burt and L. Bellantoni, MAFIA and Microwave Studio calculations]