YACS - PROGRESSION TOWARDS ISOPARAMETRIC 2.5D FINITE ELEMENTS *

B.D. Isbarn†, B. Riemann, M. Sommer, T. Weis
TU Dortmund University (DELTA), Center for Synchrotron Radiation, Dortmund, Germany

Abstract

YACS is a 2.5D finite element method solver capable of solving for the full 3D eigenfrequency spectra of resonant axisymmetric structures while reducing the computational problem to a 2D rotation plane. Prior studies and benchmarks, comparing YACS to well known commercial 3D and 2D applications, already demonstrated its capabilities of performing fast optimizations of geometries, due to its minimal computational overhead. However, because of the first order elements and basis functions used for approximation of the domain and field, this solving speed advantage vastly diminishes when targeting higher accuracies. In order to circumvent these issues, YACS was upgraded to support arbitrary order basis functions and curved meshes, leading to, but not limited to, isoparametric finite elements. This led to distinct performance and convergence improvements, especially when considering curved geometries, ideally representable by a polynomial mapping, e.g. when choosing a cavity geometry parametrization based on splines.

INTRODUCTION

Despite the wealth of readily available commercial and non-commercial codes that are suitable to solve the eigenvalue problems that typically arise from the Maxwell equations in bounded domains [1, 2], only a small fraction of these codes make use of the inherent axisymmetry of typical accelerator components. Even less codes are able to utilize the axisymmetry and solve for the full non-axisymmetric 3D electrical field. In response to this, YACS, a 2.5D finite element method solver has been developed [3]. YACS is capable to solve for the full 3D eigenfrequency spectra of resonant axisymmetric RF-structures, while also utilizing state of the art numerical libraries [4–6] and, thus, offering distinct performance increases compared to 3D codes.

FIRST ORDER APPROXIMATION

Benchmark results that were presented prior [3] and showcased the performance of YACS utilizing first order approximations of the domain and field, revealed its improvable convergence behavior, compared to commercial codes that utilize higher order approximations (see Fig. 1), where the order p refers to the finite dimensional space of a quadrilateral element [7]

$$\mathbb{P}_p = \left\{ x^j y^k : 0 \leq j,k \leq p \right\} .$$

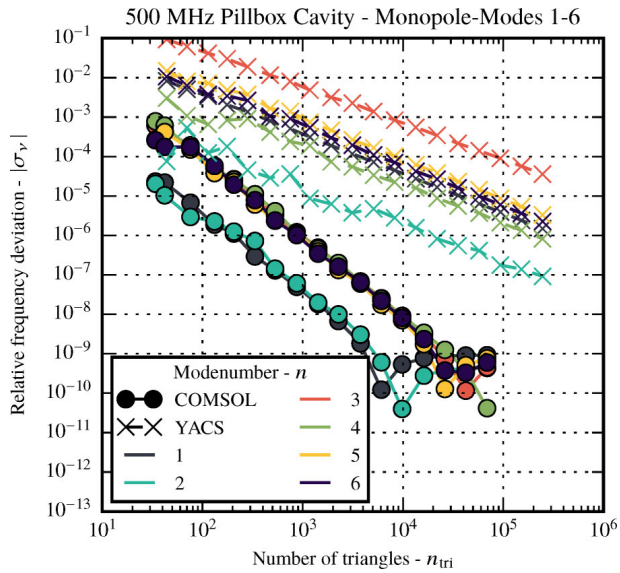

Figure 1: Relative frequency deviation of the first six monopole modes, obtained from YACS and COMSOL, of a 500 MHz pillbox cavity, as a function of the number of triangles used. The frequency deviations were calculated with respect to the analytical solution. This *older* iteration of YACS uses first order basis functions and triangles.

As a consequence, it was concluded that an increase of the order of approximation is mandatory, to be competitive in the long term. To be as flexible as possible and to enable adaptive refinement, the new implementation of YACS was required to also support arbitrary order of approximation, for both the domain and field.

ISOPARAMETRIC ELEMENTS

An isoparametric representation typically refers to an approximation of the domain and field utilizing the same basis [8]. As presented in the subsequent sections, the basis used to represent curved elements is not suitable to approximate the field. Therefore, isoparametric elements are referred to as elements that use the same order of approximation in this work. To enable maximum flexibility and adaptivity, YACS is not limited to isoparametric elements and supports superparametric and subparametric representations as well, where the order of approximation of the domain and field differs. For alleviation of development efforts, the initial implementation of the higher order approximation supports 2D problems only. Thus, all function bases are H^1-conforming.

* Work supported by the BMBF under contract no. 05K13PEB
† benjamin.isbarn@tu-dortmund.de

ISBN 978-3-95450-147-2

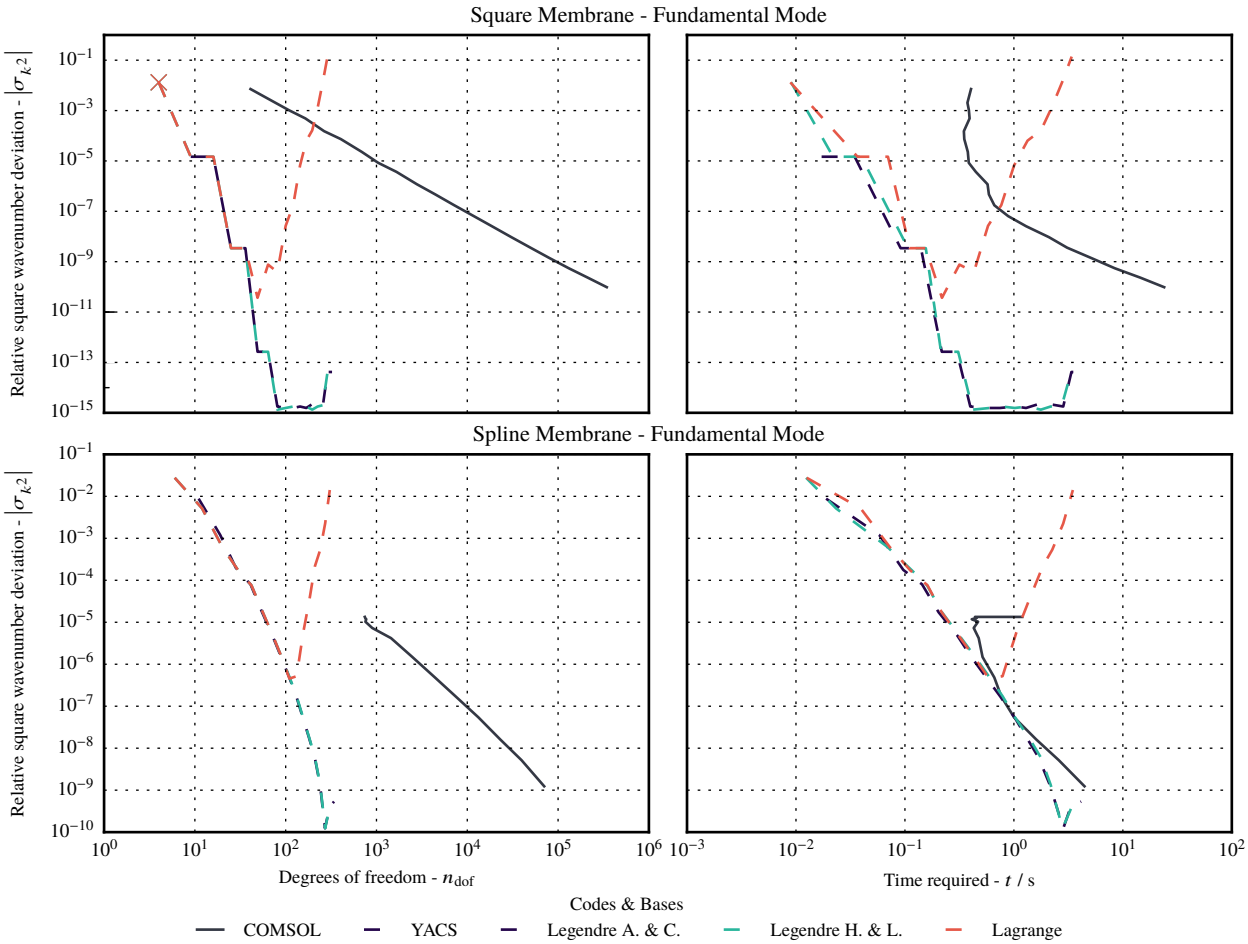

Figure 2: Relative square wavenumber deviation, obtained from YACS and COMSOL, of the fundamental mode of a square and spline membrane, as a function of the degrees of freedom and the solution time required. The wavenumber deviation were calculated with respect to the analytical solution for the square membrane, and to the COMSOL solution for the highest number of degrees of freedom for the spline membrane.

Higher Order Basis Functions

One straight forward approach to obtain a higher order basis[1]

$$\phi_i\,(x,y) = c_{ijk}\,x^{(j)}x^{(k)}\,, \tag{1}$$

is to introduce additional *virtual* points inside the reference element, and require

$$\phi_i\left(x_j,y_j\right) = \delta_{ij}\,.$$

The arising equation system leads to 2D Lagrange polynomials. One major benefit of such a function basis is that they directly connect the degree of freedom of a particular basis function ϕ_i to a physical quantity, e.g. the electrical field at the virtual point (x_j, y_j). However, there a two major drawbacks to this approach.

- The basis is not hierarchical, meaning that an increase or decrease of the order results in a completely different set of basis function. This leads to discontinuities on shared boundaries, and, thus, makes it impossible to adaptively adjust the order on an element basis.
- Using a Lagrange polynomial based function basis results in ill-conditioned system matrices, which in turn leads to diverging solutions as can be seen in Fig. 2 and 3.

Fortunately, there has been much research regarding suitable hierarchical basis functions to circumvent those issues, of which the ones proposed in [7] and [9] that utilize Legendre and integrated Legendre polynomials to construct the function basis, are presented. It should be noted that a finite basis can, according to (1), be represented by a third order coefficient tensor, so that users of YACS can easily supply their own bases.

Using the aforementioned function bases, benchmarks on a square membrane, which could be represented by a single straight edged quadrilateral element, were performed. Due to the first order quadrilateral element, the degrees of freedom

[1] Using the Einstein summation convention.

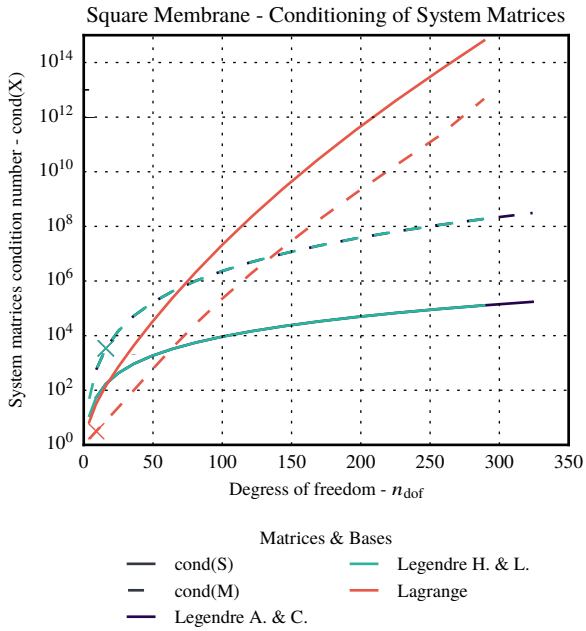

Figure 3: Condition numbers of the fundamental stiffness (S) and mass (M) matrices of the generalized eigenvalue problem for a square membrane, as a function of the degrees of freedom.

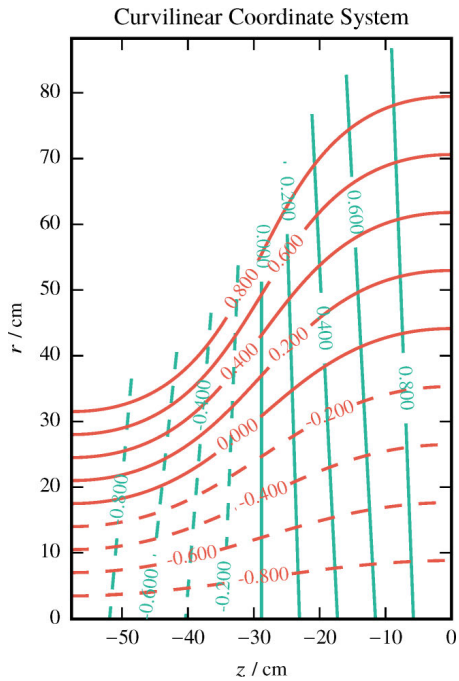

Figure 4: Curvilinear coordinate system obtained from mapping the reference quadrilateral to a spline shaped membrane. The red and green lines represent the coordinates in the reference domain.

are solely dependent on the basis order of the field approximation. Figure 2 displays the relative square wavenumber deviations as a function of the degrees of freedom and the solution time required. One can observe distinct improvements in the convergence behavior compared to the prior studies with linear basis functions, as can be seen in Fig. 1, for both the Lagrange and Legendre based basis functions. Albeit the Lagrange based basis is diverging for higher numbers of degrees of freedom, it is certainly suitable for lower order approximations.

Curved Elements

In order to minimize the geometrical error that typically arises when discretizing a curved geometry with linear resp. straight edged elements, curved elements were also implemented. The discretization of the problem domain with curved elements can be performed with Gmsh [10] and utilizes once again 2D Lagrange polynomials for the mapping between the reference element and the curved element. The benchmark results obtained from calculating the eigenvalues of a spline shaped membrane, which also has been proposed as an alternative parametrization for superconducting cavities [11], are presented in Fig. 2. Since splines offer the major benefit of being representable by a finite polynomial curve, a mapping to a curvilinear coordinate system of sufficient degree extinguishes the geometrical error. Such a curvilinear coordinate system is shown in Fig. 4.

Again, a single quadrilateral element to represent the problem domain, has been used. The degrees of freedom are, therefore, solely represented by the order of the basis of the field. The convergence behavior is similar to the benchmark results obtained from the square membrane, and outperforms the ones obtained from COMSOL [12]. However, due to the additional coordinate transformation and the overhead introduced, the computation time increases. Certainly the present implementation of curved elements can be improved, hopefully leading to substantial improvements in computation times in future iterations of YACS.

CONCLUSION

Due to the improvable convergence rates of prior iterations of YACS, compared to commercial codes, arbitrary order of approximation for both the domain and field were implemented. This led to distinct improvements in the convergence behavior. To alleviate the development efforts, this first iteration was restricted to 2D problems only. A vastly improved conditioning of the system matrices, when using preferably orthogonal basis functions, could be observed. Utilizing curved elements, the geometrical error that arises from discretizing curved problem domains could be diminished. As a result, the geometrical error for geometries that are parametrized by polynomial curves extinguishes, when choosing a suitable order of approximation. In spite of the actual improvement of the convergence behavior, the solution time required when using curved elements suffers due to the introduced overhead. The current goal for future iterations of YACS is to substantially improve the computation time when utilizing curved elements.

ISBN 978-3-95450-147-2

REFERENCES

[1] T. Rylander, P. Ingelström, and A. Bondeson, *Computational Electromagnetics*, 2nd ed., Springer New York, New York, USA, 2013.

[2] T. Wangler, *RF Linear Accelerators*, 2nd ed., Wiley-VCH, Weinheim, Germany, 2007.

[3] B.D. Isbarn, B. Riemann, M. Sommer, and T. Weis, "Yacs - A new 2.5D FEM eigenmode solver for axisymmetric RF-structures", in *Proc. IPAC'15*, Richmond, VA, USA, May 2015, paper MOPWA033, pp. 175–178.

[4] R.B. Lehoucq, D.C. Sorensen, and C. Yang, "ARPACK users guide: Solution of large scale eigenvalue problems by implicitly restarted Arnoldi methods", `http://www.caam.rice.edu/software/ARPACK/`.

[5] T.A. Davis, "Algorithm 832: UMFPACK V4.3—an unsymmetric-pattern multifrontal method", ACM Trans. Math. Software, vol. 30, no. 2, pp. 196-199, Jun. 2004.

[6] C. Sanderson, "Armadillo: An open source C++ linear algebra library for fast prototyping and computationally intensive experiments", Technical Report, NICTA, Australia, Sep. 2010.

[7] M. Ainsworth and J. Coyle, "Hierachic hp-edge element families for Maxwell's equations on hybrid quadrilateral/triangular meshes", Comput. Methods Appl. Mech. Engrg., vol. 190, no. 49–50, pp. 6709–6733, Oct. 2001.

[8] G.H. Majzoob and B. Sharifi Hamadani, "Mapping of C* elements in finite element method using transformation matrix", International Journal of Mechanical, Aerospace, Industrial, Mechatronic and Manufacturing Engineering, vol. 1, no. 1, pp. 13–16, Jan. 2007.

[9] R. Hiptmair and P.D.R. Ledger, "Computation of resonant modes for axisymmetric Maxwell cavities using hp-version edge finite elements", Int. J. Numer. Meth. Eng., vol. 62, no. 12, pp. 1652–1676, Jan. 2005.

[10] C. Geuzaine and J. Remacle, "Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities", Int. J. Numer. Meth. Eng., vol. 79, no. 11, pp. 1309–1331, May 2008.

[11] B. Riemann, T. Weis, and A. Neumann, "Design of SRF cavities with cell profiles based on bezier splines", in *Proc. ICAP'12*, Rostock-Warnemünde, Germany, Aug. 2013, paper WEP14, pp. 167–169.

[12] COMSOL Multiphysics 5.2, `http://www.comsol.com/`.