LRP 492/94 March 1994

POLLUTION FREE DISCRETIZATION OF MAXWELL'S EQUATIONS IN TERMS OF POTENTIALS

A. Jaun, K. Appert and J. Vaclavik

submitted for publication in
IEEE Transactions on Microwave Theory
and Techniques

[9] R. Gruber, F. Troyon, D. Berger, L.C. Bernard, S. Rousset, R. Schreiber, W. Kerner, W. Schneider, K.V. Roberts, "ERATO stability code", *Comput. Phys. Commun*, vol. 21, pp. 323-371, 1981

[10] C.W. Crowley, P.P. Silvester and H. Hurwitz, "Covariant projection elements for 3D vector field problems", *IEEE Trans. Magn.*, vol. 24, pp. 397-400, 1988

[11] A.F. Peterson, "Finite element solution of the vector wave equation using divergentless basis function", in *Proc. 1989 IEEE AP-S Int. Symp.*, vol. III, pp. 1624–1627

[12] K.D. Paulsen and D.R. Lynch, "Elimination of vector parasites in finite element Maxwell solutions", *IEEE Trans. Microwave Theory Tech.*, vol. MTT-39, pp. 395-404, 1991

[13] D.B. Batchelor, E.F. Jaeger and H. Weitzner, "2D full wave modeling of ICRF with finite parallel electric field", *Theory of Fusion Plasmas (Proc. Int. Workshop, Varenna, 1988) Editrice Compositori, Bologna (1988)*

POLLUTION FREE DISCRETIZATION OF MAXWELL'S EQUATIONS IN TERMS OF POTENTIALS

A. Jaun, K. Appert and J. Vaclavik

Centre de Recherches en Physique des Plasmas,
Association Euratom–Confédération Suisse,
Ecole Polytechnique Fédérale de Lausanne,
21, av. des Bains, 1007 Lausanne, Switzerland

Abstract

A 2D discretization of Maxwell's equations is studied in terms of the electromagnetic potentials using linear and cubic finite elements. The formulation is first analyzed with respect to the discrete dispersion properties to show that it is pollution free. It is then further applied to a simple cylindrical waveguide problem, showing good convergence to the analytical eigenfrequencies.

submitted for publication in
IEEE Transactions on Microwave Theory and Techniques

1 Introduction

Spectral pollution remains a major concern in wave theory when solving Maxwell's equations numerically. In waveguide calculations for example, spurious computational modes appear in the physical eigenmodes spectrum: they are generally of short wavelength comparable with the mesh size, and exhibit an electrostatic behavior. If the mesh density is increased, new parasitic modes appear in the spectrum in an unpredictable way and it is impossible to keep track of the physical solution in a convergence study.

This phenomenon has been known for some time as well among the people involved in microwave [1], fluid dynamics [2] and plasma theory [3]. Several methods have been proposed since to solve the variational problem using finite elements in more or less general cases. Grossly, they either rely on a modification of the functional, so as to "penalize" the cost of the divergence [4], [5], [6] or allow the solution to be divergence free everywhere using a modification of the finite elements basis [7], [8],[9], [10], [11]. The penalty method shifts the parasitic modes according to the size of the penalty term and leads to questions concerning the threshold sufficient to clean the region of the spectrum under study without affecting too much the physical modes [12].

Recently a new approach has been suggested to avoid pollution by solving Maxwell's equations in terms of the electromagnetic potentials [13]. No extra term has to be included into the variational problem and the discretization can be performed with standard finite elements. The computational size of the problem is increased by introducing an extra variable; the resulting Laplacian structure may however open the way to iterative resolution methods which used to fail due to the bad condition of the matrix resulting from the double-curl operator. The present work first shows that the new approach is pollution free by analyzing the 1D discrete dispersion relation arising from linear and cubic-hermite finite element discretizations on a homogeneous mesh. A formulation is then given in 2D in the case of a cylindrical waveguide and the numerical convergence to the analytical solution is studied for both types of elements.

2 Weak form in terms of potentials

A usual way of writing the time independent Maxwell's equations in terms of the electric field $\vec{E}$ results in the infamous $\nabla \times \nabla \times$ operator which is the source of pollution:

$$\nabla \times \nabla \times \vec{E} - \left(\frac{\omega}{c}\right)^2 \vec{E} = i\omega \frac{4\pi}{c^2} \vec{j}_{ext} \,. \tag{1}$$

Addition of an extra term $\eta\nabla(\nabla\cdot \vec{E})$ where η is the penalty factor, shifts the spurious modes and avoids pollution.

Examining the general vector identity $-\nabla \times \nabla \times \vec{V} + \nabla(\nabla\cdot \vec{V}) = \nabla^2 \vec{V}$ which is a similar combination of terms, it appears advantageous to use Laplacian operators. This is possible if Maxwell's equations are written in terms of the potentials $(\vec{A},\phi)$ using the Coulomb gauge:

$$\begin{cases} \nabla^2 \vec{A} + k_0^2 \vec{A} + ik_0 \nabla\phi &= -\frac{4\pi}{c} \vec{j}_{ext} \\ \nabla^2\phi - ik_0\nabla\cdot \vec{A} &= -4\pi\rho_{ext}. \end{cases} \tag{2}$$

$\omega = k_0 c$ is the circular excitation frequency and $(\vec{j}_{ext}, \rho_{ext})$ external sources chosen so as to satisfy $\nabla\cdot \vec{j}_{ext} = \rho_{ext} = 0$. Note that by taking the divergence of the first equation and combining it with the second to obtain $\nabla^2(\nabla\cdot \vec{A}) = 0$, it is clear that the Coulomb gauge is satisfied everywhere once it is imposed along the boundaries.

At this stage, it is useful to construct the variational form and to analyze the dispersion properties in the context of a finite elements discretization. This is done for the general case in a 1D slab geometry $(\vec{e_x}, \vec{e_y}, \vec{e_z})$ and assuming the dispersion to be only in $(\vec{e_x}, \vec{e_z})$. After a multiplication of Eqs.(2) by a test function $(\vec{F}^*, G^*)$ and further volume integration, the weak form is integrated by parts, keeping only the volume contributions relevant for a local analysis:

$$
\begin{aligned}
\int dV \left[-(\nabla\times \vec{F}^*)\cdot(\nabla\times \vec{A}) - (\nabla\cdot \vec{F}^*)(\nabla\cdot \vec{A}) + k_0^2\, \vec{F}^* \cdot \vec{A} + ik_0\, \vec{F}^* \cdot\nabla\phi\right] &= 0 \\
\int dV \left[(\nabla G^*)\cdot(\nabla\phi) - ik_0\nabla G^*\cdot \vec{A}\right] &= 0
\end{aligned}
\qquad (3)
$$

A finite element approximation is then performed on a homogeneous mesh $x_j = jh$ by writing

$$
(\vec{A},\phi)_w(x) \sim \sum_j e^{ikx_j}\eta_j^w(x) \qquad w = 1..4. \qquad (4)
$$

$\eta_n^w(x)$ is the basis function associated with the mesh point n and used for approximating the component $(\vec{A},\phi)_w$. Expressing the test function in terms of finite elements and carrying out the integration over their finite support, leads to a discrete dispersion relation in the form of $det(\overleftrightarrow{D}) = 0$. This is then solved analytically using a symbolic manipulation software. Choosing the numerical parameters as $h = 1$ and $k_z = 3$ finally results in a function relating the parallel refractive index $(\frac{\omega}{k_z c})^2$ to the precision of the numerical discretization kh.

Fig.1 shows a comparison for linear elements between the standard polluted scheme Eq.(1) leading to the three solutions (a,b,d) and the new scheme Eqs.(2) which has a degenerated set of solutions (d,d,e). Pollution is present in two branches. The first (a) corresponds to a short wavelength mode, propagatory below the cutoff frequency. The second results from the double valued solution (b) which allows, for a given frequency, the coexistence of two modes. Here again, one of the solutions has a short wavelength comparable with the mesh size. Note that a solution (e) exists for high frequencies and short wavelengths. It is an unphysical electrostatic mode ($\phi \neq 0$) which does not satisfy $\nabla\cdot \vec{A}= 0$. It can however not be excited if the Coulomb gauge is properly imposed so that (d) remains the only branch approximating (c), showing at the same time that Eqs.(2) discretized with linear elements are pollution free. The same analysis is repeated using cubic elements in Fig.2.

Confident of the local properties of the new scheme, we continue with the formulation of a driven global problem in a specific geometry. Although our aim is to model the wave

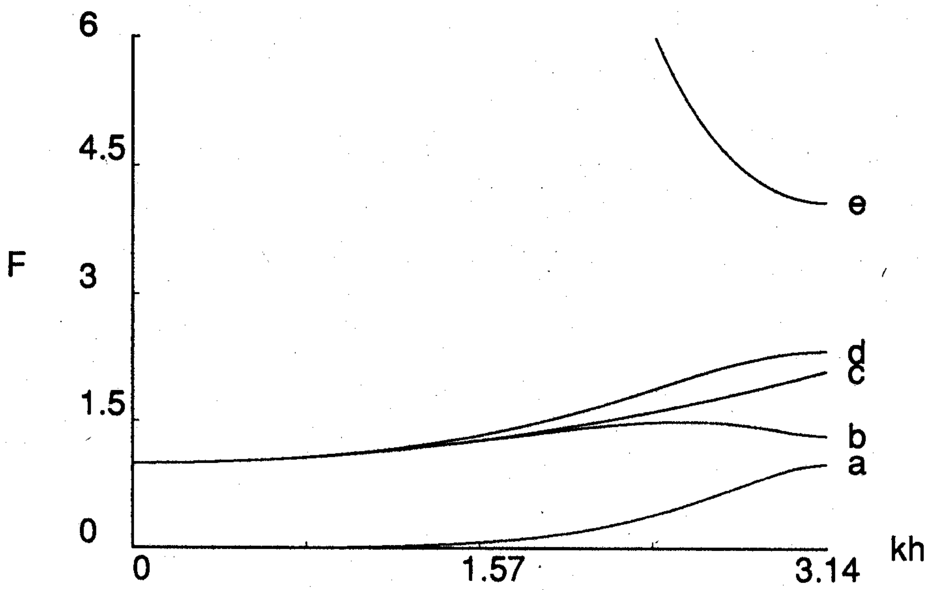

Figure 1: *1D discrete dispersion relation* $F = (\frac{\omega}{k_z c})^2$ *as a function of kh using linear elements. While (c) reproduces the analytical solution, the polluted scheme Eq.(1) leads to solutions (a,b,d), and the new method Eqs.(2) to (d,d,e).*

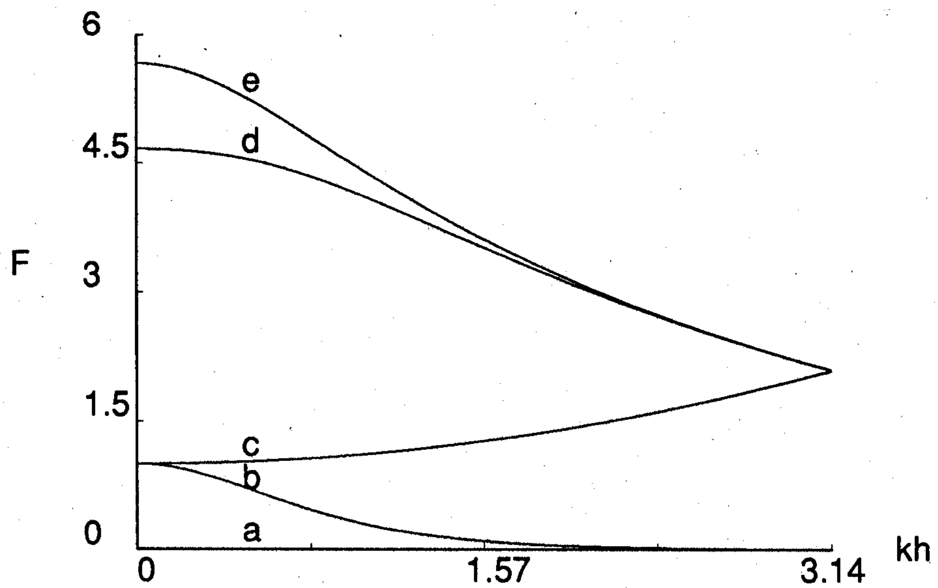

Figure 2: *1D discrete dispersion relation* $F = (\frac{\omega}{k_z c})^2$ *as a function of kh using cubic elements. While (c) reproduces the analytical solution, the polluted scheme Eq.(1) leads to solutions* $(a \equiv 0, b, b, c, d, e)$*, and the new method Eqs.(2) to (c,c,c,e,e).*

propagation in a toroidal fusion device, we restrict here our analysis to a 2D cylindrical waveguide in polar geometry $(\vec{e_\rho}, \vec{e_\theta}, \vec{e_z})$. Assuming the third coordinate being ignorable, the variational problem is constructed directly from Eqs.(2), along the same lines as for Eqs.(3). Regularity is enforced after partial integration, canceling the surface contribution of the cylinder axis. As mentioned above, the gauge condition $\nabla\cdot \vec{A}= 0$ imposed on the surface term at the cylinder boundary, is sufficient to select in a least squares sense the proper gauge in the whole domain. The complete expression finally reads:

$$
\begin{aligned}
&\int_0^{2\pi} d\theta \int_0^a \rho d\rho \Big\{-(\tfrac{1}{\rho}\tfrac{\partial F_z^*}{\partial \theta} + ik_z F_\theta^*)(\tfrac{1}{\rho}\tfrac{\partial A_z}{\partial \theta} - ik_z A_\theta) + (ik_z F_\rho^* + \tfrac{\partial F_z^*}{\partial \rho})(ik_z A_\rho - \tfrac{\partial A_z}{\partial \rho}) \\
&-(\tfrac{1}{\rho}\tfrac{\partial}{\partial \rho}(\rho F_\rho^*) + \tfrac{1}{\rho}\tfrac{\partial F_\theta^*}{\partial \theta} - ik_z F_z^*)(\tfrac{1}{\rho}\tfrac{\partial}{\partial \rho}(\rho A_\rho) + \tfrac{1}{\rho}\tfrac{\partial A_\theta}{\partial \theta} + ik_z F_z^*) + ik_0(F_\rho^* \tfrac{d\phi}{\partial \rho} + \tfrac{1}{\rho}F_\theta^* \tfrac{\partial \phi}{\partial \theta} + ik_z F_z^* \phi) \\
&-(\tfrac{1}{\rho}\tfrac{\partial}{\partial \rho}(\rho F_\theta^*) - \tfrac{1}{\rho}\tfrac{\partial F_\rho^*}{\partial \theta})(\tfrac{1}{\rho}\tfrac{\partial}{\partial \rho}(\rho A_\theta) - \tfrac{1}{\rho}\tfrac{\partial A_\rho}{\partial \theta}) + k_0^2(F_\rho^* A_\rho + F_\theta^* A_\theta + F_z^* A_z)\Big\} = \\
&-\tfrac{4\pi}{c}\int_0^{2\pi} d\theta \int_0^a \rho d\rho \left\{F_\theta^* j_{ext,\theta} + F_z^* j_{ext,z}\right\}
\end{aligned}
$$

$$
\begin{aligned}
&\int_0^{2\pi} d\theta \int_0^a \rho d\rho \Big\{-(\tfrac{\partial H^*}{\partial \rho}\tfrac{\partial \phi}{\partial \rho} + \tfrac{1}{\rho^2}\tfrac{\partial H^*}{\partial \theta}\tfrac{\partial \phi}{\partial \theta} + k_z^2 H^* \phi) - ik_0 H^*(\tfrac{1}{\rho}\tfrac{\partial}{\partial \rho}(\rho A_\rho) + \tfrac{1}{\rho}\tfrac{\partial A_\theta}{\partial \theta} + ik_z A_z)\Big\} \\
&+\int_0^{2\pi} d\theta \rho \left\{ik_0 H^* A_\rho - H^* \tfrac{\partial \phi}{\partial \rho}\right\} = 0
\end{aligned}
\tag{5}
$$

Prior to the resolution of the discretized Eqs.(5) it is necessary to impose the proper behavior of the solution on the domain boundaries. Unicity has to be required on the cylinder axis where a finite number of discrete values of the potentials degenerate to one:

$$
\begin{cases}
A_x = & A_\rho^i(\vec{e_\rho}\cdot\vec{e_x}) + A_\theta^i(\vec{e_\theta}\cdot\vec{e_x}) & = const \\
A_y = & A_\rho^i(\vec{e_\rho}\cdot\vec{e_y}) + A_\theta^i(\vec{e_\theta}\cdot\vec{e_y}) & = const \\
A_z = & A_z^i & = const \\
\phi = & \phi^i & = const \qquad \forall i = 1..N_\theta
\end{cases}
\tag{6}
$$

For a perfectly conducting waveguide, the boundary conditions result in vanishing scalar and tangential vector potentials

$$A_\theta^i = 0 \quad A_z^i = 0 \quad \phi^i = 0 \tag{7}$$

$$(\tfrac{\partial A_\theta}{\partial \theta})^i = 0 \quad (\tfrac{\partial A_z}{\partial \theta})^i = 0 \quad (\tfrac{\partial \phi}{\partial \theta})^i = 0 \qquad \forall i = 1..N_\theta \tag{8}$$

Eqs.(8) have to be specified only for cubic elements.

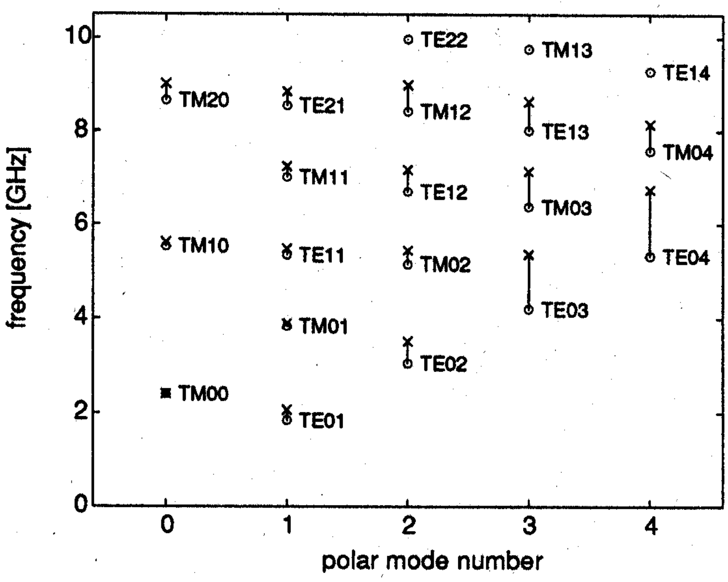

Figure 3: *Theoretical (circles) and numerical (x-marks) eigenfrequencies using linear elements*

3 Results

In order to validate the formulation numerical computations are performed in 2D for a vacuum cylinder, so that the result can easily be compared with the well known analytical solution.

For the driven problem under discussion, all fundamental eigenmodes can be excited by an arbitrary spatial distribution of the source current by proper tuning of the antenna frequency $f = \frac{\omega}{2\pi}$ which is chosen with a small imaginary part. Scanning in frequency and identifying the mode structure corresponding to the peaks of the electromagnetic energy, the numerical solution can be compared with the analytical theory. Fig.3 shows the eigenfrequency spectrum consisting of transverse electric TE_{lm} and transverse magnetic TM_{lm} modes obtained using linear finite elements on a homogeneous mesh 8x8, for polar mode numbers up to $m = 4$. This corresponds to the discretization limit of 2 mesh points per polar wavelength. Note that no solution has been found below the fundamental eigenfre-

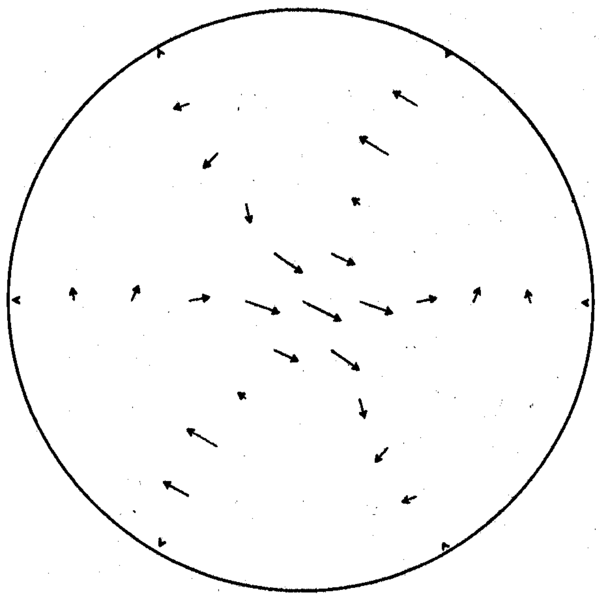

Figure 4: *Cubic-hermite solution for* $\vec{A}_\perp$ *for an eigenmode* TE_{11}

quency of the mode TE_{01}; as expected from the local analysis, the new scheme has no spurious modes related to the branches (a) of Fig.1 or (b) of Fig.2. For higher frequencies, the electrostatic short wavelength modes related to (e) have also properly been suppressed. All together, this shows that the new scheme is pollution free.

Fig.4 shows the structure of the vector potential in the case of an eigenmode TE_{11} calculated with bicubic finite elements on a homogeneous grid 6×6. Considering the relatively coarse resolution, the value of the eigenfrequency obtained numerically $f^{num} = 5.3323$ [GHz] is in excellent agreement with the analytical result $f^{th} = 5.3314$ [GHz].

The quality of the discretization is best judged in a convergence study monitoring the relative error in the eigenfrequency and the precision of the gauge condition as a function of the number of mesh intervals. Fig.5 shows the convergence of the relative eigenfrequency deviation $\Delta\omega = \frac{\omega^{num}-\omega^{th}}{\omega^{th}}$ for the eigenmodes TE_{02}, TE_{01}, TE_{11} and TM_{00}. Using linear elements $\Delta\omega$ decreases quadratically. With cubics it reaches a convergence law near to the fifth power of the number of mesh intervals, with an excellent initial precision better than

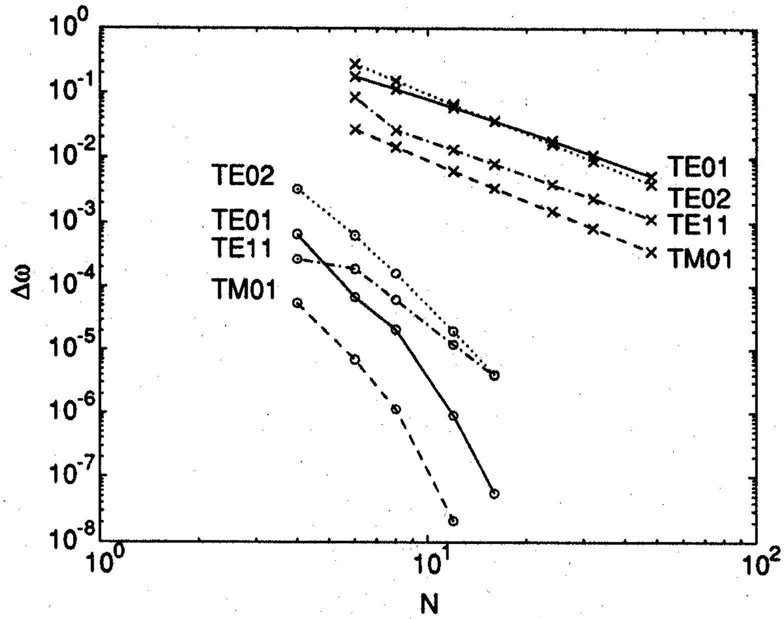

Figure 5: *Relative frequency deviation* $\Delta\omega$ *versus the number of mesh intervals* N *for the eigenmodes* TE_{01}, TE_{02}, TE_{11}, TM_{00} *using linear (x-marks) and cubic (circles) elements*

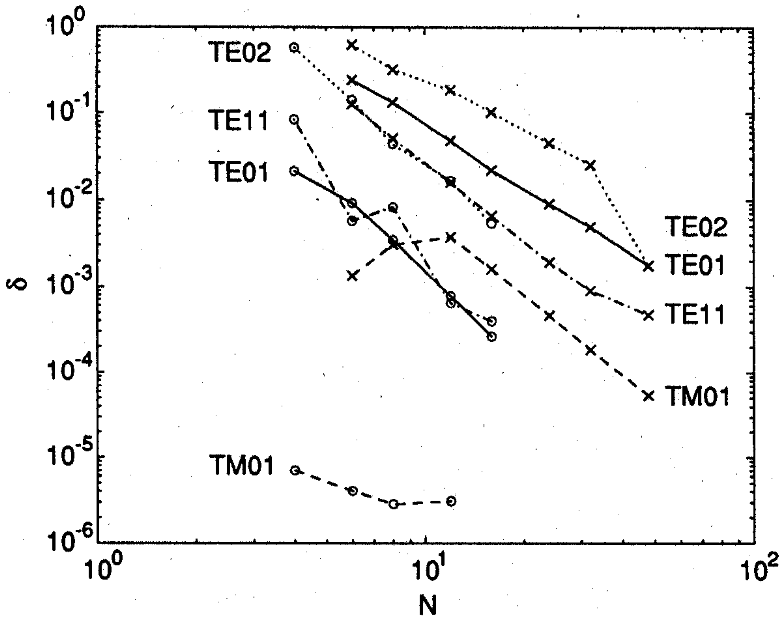

Figure 6: *Precision of the gauge* δ *versus the number of mesh intervals* N *for the eigenmodes* TE_{01}, TE_{02}, TE_{11}, TM_{00} *using linear (x-marks) and cubic (circles) elements*

1% for two mesh points per wavelength. It is interesting to note the slight degradation of the convergence rate for the eigenmodes TE_{l1}. This phenomenon has to do with the finiteness of the solution on the cylinder axis which interferes with the natural boundary condition which selects only the regular solution for $\rho \rightarrow 0$.

As expected from considerations above, convergence is also achieved globally for the gauge condition $\nabla \cdot \vec{A} = 0$. Compared here with a typical variation of the field and averaged over the volume, we define the factor $\delta = \langle \frac{a|\nabla \cdot \vec{A}|}{|\vec{A}|} \rangle$ related to the precision of the gauge. Fig.6 shows a quadratic/quartic convergence of δ with linear/cubic elements respectively.

Although a cubic finite elements discretization is much heavier to implement as far as the programming is concerned, the computer time required to achieve a precision around 1% in the eigenfrequency is already 2-4 times smaller with cubic than with linear elements. The situation is even more pronounced for higher precisions, as cubic elements have a higher convergence rate than linear elements.

As a final remark, and to emphasize on the robustness of the method, we note that the formulation presented in this paper has been extended successfully to the curvilinear geometry of a tokamak equilibrium to simulate the linear wave propagation in a cold toroidal plasma. Results related to that work will be reported elsewhere.

4 Conclusion

A 2D discretization of Maxwell's equations in terms of the electromagnetic potentials has been shown to be pollution free using standard linear or cubic-hermite finite elements. Analyzing the dispersion properties of the discrete problem, it was possible to identify the spurious branches in the standard approach and to show that the new method does not suffer from pollution. A formulation has been given for a 2D cylindrical waveguide, showing good convergence to the analytical solution for both types of elements. The excellent precision achieved with cubic elements already for coarse mesh densities makes them very attractive for global modes simulations.

Acknowledgment

This work was supported in part by the Swiss National Science Foundation.

References

[1] Z.J. Cendes and P.P. Silvester, "Numerical solutions of dielectric loaded waveguides: I-Finite element analysis", *IEEE Trans. Microwave Theory Tech.*, vol. MTT-18, pp.1124-1131, 1970

[2] P.A.Raviart, "Hybrid finite element methods for solving 2nd order elliptic equations", *Conf. on Numerical Analysis, Royal Irish Academy, Dublin*, 1974

[3] K. Appert, D. Berger, R. Gruber, F. Troyon, and J. Rappaz, "Studium de Eigenschwingungen eines zylindrichen Plasmas mit der Methode der finiten Elemente", *J. Appl. Math. Phys. (ZAMP)* vol. 25 pp. 229-240, 1974

[4] B.M.A. Rahman and J.B. Davies, "Penalty function improvement of waveguide solutions by finite elements", *IEEE Trans. Microwave Theory Tech.*, vol. MTT-32, pp. 922-928, 1984

[5] M. Koshiba, K. Hayata and M. Suzuki, "Finite element formulation in terms of the electric field vector for electromagnetic waveguide problems", *IEEE Trans. Microwave Theory Tech.*, vol. MTT-30, pp. 900-905, 1985

[6] X. Llobet, K. Appert and J. Vaclavik, "A modified electromagnetic wave equation", in *Theory of Fusion Plasmas (Proc. Int. Workshop, Varenna, 1990) Editrice Compositori, Bologna (1990)*

[7] K. Appert, D. Berger, R. Gruber and J. Rappaz, "A New finite element approach to the normal mode analysis in magnetohydrodynamics", *J. Comp.Phys.*, vol. 18, pp. 284-299, 1975

[8] P.A.Raviart and J.M.Thomas, "Primal hybrid finite element methods for 2nd order elliptic equations", *Math. Comp.* vol. 31 pp.391-413, 1977

(14)