On the convergence of 2D and 3D finite element/ boundary element analysis for periodic acoustic waveguides

William Daniau, Michel Lenczner, Thierry Laroche, Julien Garcia, Emile Carry, Sylvain Ballandras
Institut FEMTO-ST, UMR 6174 CNRS-UFC-ENSMM-UTBM, Dépt Temps-Fréquence,
25030 Besançon Cedex, France

william.daniau@femto-st.fr

Abstract: **Finite Element Analysis/Boundary Element Methods (the so-called FEA/BEM) are a key-tool for the simulation of elastic waveguides and transducers used for the design of RF filters, sources and sensors. We analyze the optimal convergence conditions of corresponding computations, showing the interest of 2nd degree interpolation to improve both the accuracy and the delay of such calculations. We also propose a general and efficient approach to integrate boundary integrals of 3D problems, allowing to minimize the computation delay of the BEM part, the most costly of the whole model.**

I- Introduction

The interest of simulation tools based on the combination of finite element analysis and boundary element method (FEA/BEM) now has been well established for the analysis of periodic waveguide properties. The flexibility of FEA is particularly well-suited to simulate interfaces exhibiting complex shapes involving materials of different nature whereas the BEM approach provides an accurate description of the susbtrate, whatever its composition (semi-infinite media, finite thickness plates, stacks) assuming flat interfaces. It can be performed in 2D and 3D, accounting for acoustic and dielectric losses. Compared to the approach promoted by Ventura [1] where finite elements only are used to compute the acoustic contribution of the electrodes, the computation delay of our method still appears as its main flaw.

As a consequence, the possibility to improve the convergence and to optimize the computation delay of periodic FEA/BEM has been investigated. We particularly focus on the use of high accuracy finite elements to address the problem. We have considered the case of 4-degree-of-freedom 2D and 3D elements to compute the harmonic admittance of Rayleigh-type Surface Acoustic Wave (SAW) on AT-X quartz and shear-polarized leaky wave trapped on Y+42° $LiTaO_3$ under thick electrode grating. For 2D analysis, we have used the Lagrange interpolation scheme to develop finite and boundary elements up to the third degree. For 3D analysis, we only have considered first and second degree polynomials for both finite and boundary elements. However, in that latter case, contrarily to what proposed by Wilm et al [2], we have developed an approach based on non isoparametric boundary elements, as the radiation interface always must remain flat. This approach allows for a dramatic gain in computation delay without any loss in accuracy.

In both cases, calculation details are explained in details and the corresponding implementation is illustrated by comparing numerical results for the above mentioned case studies. It is found that the degree of interpolation polynomials plays an important role in the convergence velocity. For instance, 2D analysis achieved with 2nd degree polynomials for Rayleigh waves converges 4 times faster than using 1st degree interpolation. We also observe less dramatic gains when increasing the polynomials degree. The limit of the approach is emphasized in terms of accuracy/convergence delay/elementary matrix size trade-off.

II- 2D Interpolation issues

Since more than 15 years now we develop in our group a software called TRPP3D based on a mixed Finite Element Analysis and Boundary Element Method, the so-called FEA/BEM analysis allowing the simulation of any periodic structure radiating into any stratified layer. It is not the purpose of this paper to describe the basis of FEA/BEM, this can be found in many references [1-4], nevertheless its principle is summarized in Fig. 1 for the case of an inter-digital transducer on a single piezoelectric material. This kind of approach exploits two main features : considering periodic structures allows for reducing the FEA part of the model to the very minimum (i.e. the inhomogeneous region within a single period), and as acoustic radiations are taken into account by Green's functions, only a very small part of the substrate needs to be meshed.

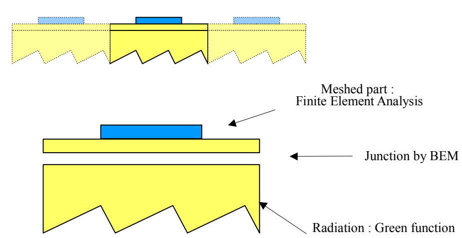
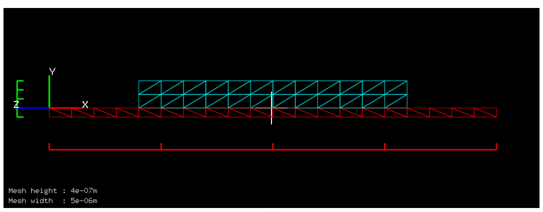


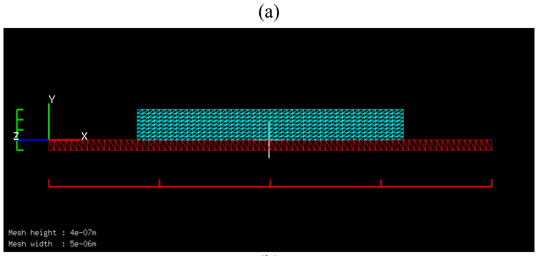
Figure 1 : Typical structure and principle of the FEA/BEM approach for the simulation of periodic elastic wave transducers

In our software, elements using 1st and 2nd degree polynomials are both implemented for the Lagrange interpolation, however it was not obvious which one should be preferred to address the simulation of acoustic waveguides. We used to adopt 1st degree interpolation to reduce computation durations and 2nd degree polynomial to improve the computation accuracy, as the displacement and potential solutions should be continuous in the whole computation domain.

At first glance, it sounds obvious that for a given number of elements, the use of 1st degree interpolation favors the computation speed, but until now we did not establish an objective criterion to emphasize the impact of the interpolation degree on the model accuracy. To address this issue, we have considered the simple problem of a Rayleigh wave propagating under an infinite periodic aluminum electrode grating on (AT,X) quartz. 1st and 2nd degree interpolation then was used to compute the harmonic admittance of the corresponding transducer structure. The mesh density is characterized by the number of radiating elements, as it conditions the size of the final FEA/BEM linear system to solve [5] and hence the computation delay and accuracy as well. Figures 2(a,b) show two examples of the implemented meshes (for 20 and 80 radiating elements respectively). When increasing the number of radiating elements, we also made the aluminum electrode mesh denser to avoid abnormally stretching the elements (i.e. length/width smaller than 3).



(a)



(b)

Figure 2 : Examples of the implemented meshs for assessing the intrication between computation delay and accuracy, the blue domain corresponds to the aluminum electrode, the red one is a thin layer of subtrate connecting FEA with BEM, p=5µm, a/p=0.6, h/2p=3%
(a) 20 radiating elements (b) 80 radiating elements

Figure 3 shows the calculated imaginary part of the harmonic admittance using 1st degree interpolation whereas Fig. 4 shows the same result obtained using 2nd degree interpolation. In both cases, as expected, the resonance frequency first is overestimated but the calculation tends to converge toward the exact solution when the mesh density increase. From theses results, we easily deduce first that the calculation convergence is obviously much faster for the 2nd degree interpolation analysis than for the 1st degree one. We also show that with only 10 radiating elements using 2nd degree interpolation elements, the accuracy is the same than the one obtained with 80 radiating elements for 1st degree interpolation elements.

The relative accuracy and calculation delay are plotted on Fig.5 for both 1st and 2nd degree interpolation elements versus mesh density, represented by the number of radiating elements as stated above. It emphasizes what was first expected, i.e. for a given mesh density, 2nd degree interpolation is more accurate, and 1st degree interpolation yields faster computations. However, plotting the relative accuracy of the results versus computation delay learns more about the optimal computation configuration. Figure 7 clearly shows that for a given calculation time, the accuracy is always better using 2nd degree interpolation than using 1st degree one.

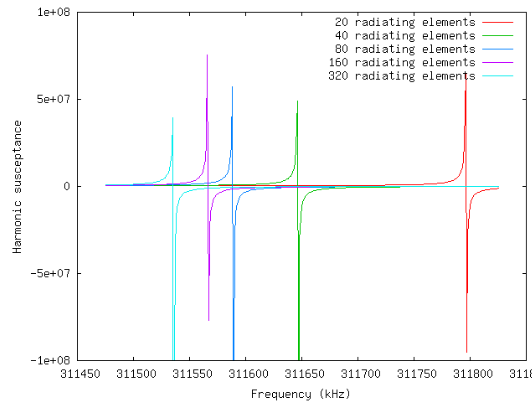


Figure 3 : Harmonic susceptance vs frequency computed using 1st degree interpolation elements

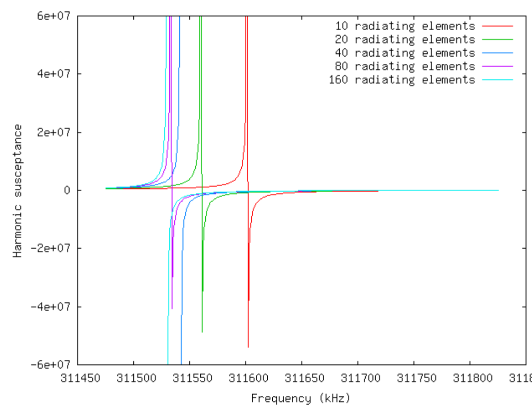


Figure 4 : Harmonic susceptance vs frequency computed using 1st degree interpolation elements

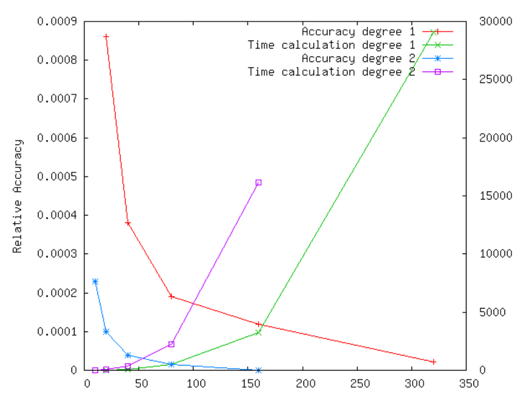


Figure 5 : Calculation time and relative accuracy vs mesh density (number of radiating elements)

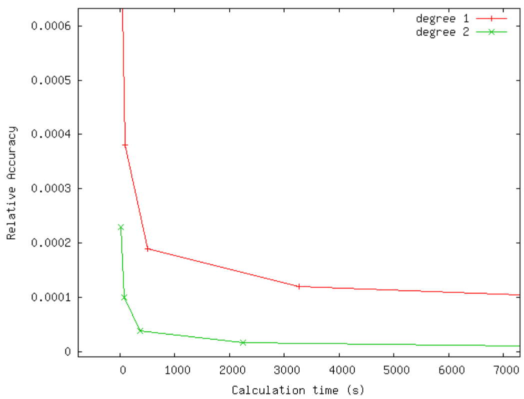


Figure 6 : Comparison between accuracy/calculation delay relations for 1st and 2nd degree interpolation elements

As a conclusion of this section, we can reliably consider that it is always a better choice to use 2nd degree interpolation elements rather than 1st degree, whether fast computations or accurate results are looked for.

III- 3D BEM INTEGRATION

A. Position of the problem

In 3D, the boundary elements are 2D elements corresponding to the faces of the 3D elements, i.e. in our case triangles or quadrangles. This will be referred as "element" in what follows. One part of the implementation of the periodic boundary elements consists in calculating many double sum integrals such as

$$\iint_{Real\,element} P_n(x,y)\, e^{-2j\pi(\alpha x+\beta y)}\, dx\, dy \quad (1)$$

where P_n represent one of the interpolation polynomials in the real element coordinates. However, calculating this sum over the real element is not an option as describing the integration bounds of a general triangle or quadrangle is not an easy task. This means that this operation must be achieved in the reference element [6] which is perfectly in accordance with the finite element method. This yields

$$\iint_{Reference\,element} J(\eta,\xi)\, P_{n\,Ref}(\eta,\xi) \cdot e^{-2j\pi P_{\exp}(\eta,\xi)}\, d\eta\, d\xi \quad (2)$$

where P_{nRef} represents one of the interpolation polynomials in the reference element (which are then perfectly known), η and ξ are the coordinates in the reference system of axes and J represents the geometrical transformation's jacobian [6]. The exponential argument is now a new polynomial P_{exp}. Note that we can state that P_{nRef} and P_{exp} are polynomials as we consider the geometrical transformation to be also polynomial (which is the case in the finite element method [6]).

The first approach that has been implemented in our software consisted in performing numerical integration. This was done using a Gauss-Kronrod adaptative method (adapted from netlib's quadpack for double sum), providing reliable and accurate results [2]. However, it rapidly turned out that this approach was not really efficient as this part of the calculation was taking quite a lot of time. This can be explained as follows. The number N of integrations to be performed for the BEM part is given by

$$N=\gamma_x \gamma_y h_x h_y e\, n \quad (3)$$

where γ_x and γ_y represent respectively the number of γ excitation parameter on both axes x and y defining the radiating surface, h_x and h_y the number of harmonics for the calculation of the Green's function on both axes, e represents the number of radiating elements and n the number of integration polynomials on the element. If we consider a very small case where the radiating surface is composed of 100 elements (10 on each axes), 8 integration polynomials, 20 harmonics on each axes and only 1 excitation parameter, this will give us N=1 280 000. Now each sum requires a certain number of function evaluations, for example using a 15 points Gauss-Legendre integration will need 225 functions evaluations (15^2) which leads to a total of 288 000 000 (note that this is even worse with the Gauss-Kronrod method which needs a minimum of 484 function evaluations). One then can easily understand the penalizing nature of this approach.

B. Analytical solution

As it is stated in reference [7], integrals of functions of several variables, over regions with dimension greater than one, are "*not easy*" and it always involves a lot of function evaluations. Consequently, we have tried to use an other approach consisting in using an analytical solution of equation (2). However this solution only exist if the degree of the polynomial P_{exp} is 1. This analytical solution is given by equation (4) [8] for the case of a one variable function. $P^{(k)}$ represent the k-th derivative of the degree m polynomial P_m.

$$\int P_m(x)\, e^{ax}\, dx = \frac{e^{ax}}{a} \sum_{k=0}^{m} \frac{P^{(k)}(x)}{a^k} \quad (4)$$

The degree of P_{exp} will only be 1 if the geometrical transformation that is used between the real element and the reference element is linear. The elements we use in our software are iso-parametric, which means that the geometrical transformation is described by the same polynomials that are used for interpolation. The initial approach consisted to use this "natural" transformation, but the only case for which this transformation is linear corresponds to the 3-node triangle element (i.e. 1st degree Lagrange interpolation polynomials). In our new approach, we then do not use this transformation but a linear one. This is an acceptable approximation as the radiating surface in our model has to be a plane.

C. Linear Transformation

We first consider the case of triangle elements. As previously emphasized, the transformation corresponding to 1st degree Lagrange interpolation is linear, we then use it for all our triangle elements whatever their interpolation degree is. In finite element formalism [6], the transformation allows to easily transform coordinates from the reference element to the real ones, this is given by equation (5) where x_i,y_i represent the coordinates of the 3 summits of the triangle in real coordinates :

$$[x\ y]=[1-\xi-\eta\quad \xi\quad \eta]\begin{bmatrix} x_1 & y_1 \\ x_2 & y_2 \\ x_3 & y_3 \end{bmatrix} \quad (5)$$

once developed this expression gives (6) :

$$\begin{cases} x=(x_2-x_1)\xi+(x_3-x_1)\eta+x_1 \\ y=(y_2-y_1)\xi+(y_3-y_1)\eta+y_1 \end{cases} \quad (6)$$

The Jacobian matrix *MJ* is given by (7)

$$MJ=\begin{bmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{bmatrix}[x\ y]=\begin{bmatrix} x_2-x_1 & y_2-y_1 \\ x_3-x_1 & y_3-y_1 \end{bmatrix} \quad (7)$$

and the Jacobian J, determinant of the Jacobian matrix is given by (8)

$$\begin{aligned} J=x_1 y_2-x_1 y_3+x_2 y_3 \\ -x_2 y_1+y_1 x_3-y_2 x_3 \end{aligned} \quad (8)$$

Note that for this linear transformation, J is a constant representative of the current element and that can be taken outside the integral. Now we come back to our formulation of equation (2). As summarized in Fig.7, the procedure is rather easy: the archetypal interpolation polynomials (whatever their degree) are considered in the reference element, the jacobian is given by (8) and $P_{exp}(\xi,\eta)$ is obtained by inserting (6) in $\alpha x+\beta y$ which gives the expression in (9) (of 1st degree)

$$\begin{aligned} P_{\exp}(\xi,\eta)=(\alpha(x_2-x_1)+\beta(y_2-y_1))\xi \\ +(\alpha(x_3-x_1)+\beta(y_3-y_1))\eta+\alpha x_1+\beta y_1 \end{aligned} \quad (9)$$

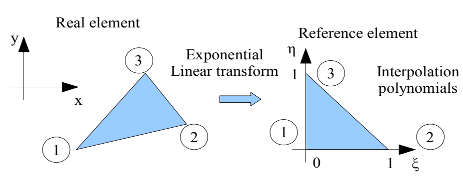


Figure 7 : FEA transformation of the linear triangle from real to reference coordinates

For the quadrangle, things are more complicated as a linear transformation for 4 points does not mathematically exists. The methodology developed in that case is summarized in Fig.8. The calculation of the sum is achieved over two "pseudo" triangle reference elements. Each quadrangle is divided into two triangles (1 4 2) and (3 2 4). The exponential part P_{exp} is obtained into each triangle using the previously described linear transformation. Concerning the interpolation polynomials, they are known into the "true" quadrangle reference element. We then need to find their expressions into the two "pseudo" triangle reference elements. This is done using the expression of the transformation between the reference quadrangle and the two triangles given by (10) and (11).

$$Triangle\,1:\begin{cases} \xi=\dfrac{1+\xi_c}{2} & \xi_c=2\xi-1 \\ \eta=\dfrac{1+\eta_c}{2} & \eta_c=2\eta-1 \end{cases} \quad (10)$$

$$Triangle\,2:\begin{cases} \xi=\dfrac{1-\xi_c}{2} & \xi_c=1-2\xi \\ \eta=\dfrac{1-\eta_c}{2} & \eta_c=1-2\eta \end{cases} \quad (11)$$

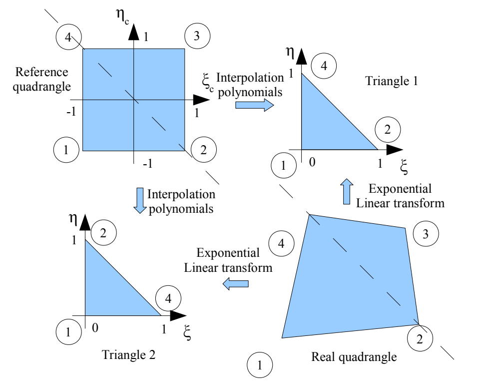


Figure 8 : FEA transformation of the linear quadrangle from real to reference coordinates via 2 pseudo-triangles

D. Implementation

Once all the principles have been set, we enter the implementation process. After examining all the possible polynomials (corresponding to triangle and quadrangle Lagrange degree 1 and 2), the general expression of the integrals to compute is given by (12)

$$\begin{aligned} \int_{\xi=0}^{1}\int_{\eta=0}^{1-\xi}\Big(a_1+a_2\xi+a_3\eta+a_4\xi^2+ \\ a_5\xi\eta+a_6\eta^2+a_7\xi^2\eta+a_8\xi\eta^2\Big). \\ e^{-2j\pi(\theta_1\xi+\theta_2\eta+\theta_3)}d\xi\, d\eta \end{aligned} \quad (12)$$

Even if the analytical solution for this sum exists, its expression if far two long to be written here. We have used the commercial software Maple to derive this expression. Furthermore, Maple allows the generation of Fortran code for implementing this expression, which has been used for practical coding. After final implementation we have gain more than two orders of magnitude in the calculation time, with absolutely no significant differences.

IV- Conclusion

We have proposed an analysis of the accuracy/computation speed conditions of 2D FEA/BEM analysis of infinite 1-D periodic transducers. It turns out that 2nd degree polynomials used to interpolate the physical unknowns of the problem always yield the best trade-off in terms of calculation delay for a given accuracy (and vice-versa). This work will be extended soon to higher degree interpolations for definitely find out the optimal interpolation configuration in terms of accuracy/delay. We also have proposed a pragmatic approach for integrating BEM integrals for 3D periodic FEA/BEM computations. The proposed approach allows for gaining two orders of magnitude in computing the integrals of the BEM part of the model. Next work will be dedicated to find out the best trade-off for accuracy/computation delay for 3D problems as what has been achieved here in 2D.

References

[1] P. Ventura & al, "Combined FEM and Green' s function analysis of periodic SAW structure, application to the calculation of reflection and scattering parameters", Trans. on UFFC, Vol. 48, n°5, pp. 1259-1274, 2001

[2] M. Wilm & al, "Three-dimensional modeling of micro-machined-ultrasonic-transducer arrays operating in water", Ultrasonics, Vol. 43, Issue 6, May 2005, Pages 457-465

[3] H. Reichinger, A.R. Baghai-Wadji, "Dynamic 2D analysis of SAW devices including massloading", Proc. of the IEEE Ultrasonics Symposium, pp. 7-10, 1992.

[4] G. Endoh, K. Hashimoto, M. Yamagushi, "SAW propagation characterization by finite element method and spectral domain analysis", Jpn. J. Appl. Phys., 34, 5B, pp. 2638-2641, 1995

[5] S. Ballandras, R. Lardat, M. Wilm, Th. Pastureaud, A. Reinhardt, N. Champavert, W. Steichen, W. Daniau, V. Laude, R. Armati, G. Martin, "A mixed finite element/boundary element approach to simulate complex guided elastic wave periodic transducers", Journal of Applied Physics, Volume 105, Issue 1, pp. 014911-014911-10 (2009)

[6] O. C. Zienkiewicz, R. L. Taylor, J. Z. Zhu, "The finite element method, its basis and fundamentals" sixth edition, Elsevier.

[7] William H. Press, Saul A. Teukolsky, William T. Vetterling, Brian P. Flannery, "Numerical Recipes in Fortran 77" second edition, Cambridge University Press.

[8] I. S. Gradshteyn, I. M. Ryzhik, "Table of integrals series and products " fourth edition, Academic Press.