XLI CILAMCE
XLI Ibero-Latin American Congress on Computational Methods in Engineering
16-19 November, 2020 FOZ DO IGUAÇU PARANÁ – BRAZIL

Uniform FEM B-Splines in the analysis of free vibration problem in the axisymmetric nano shells in elastic medium using a non-local elasticity theory

Oscar A. Garcia [1], Rodrigo Rossi [1]

[1] *Depto. de Engenharia Mecânica, Universidade Federal do Rio Grande do Sul*
Sarmento Leite 425, 90050-070, Porto Alegre/RS, Brazil
oagsuarez@gmail.com, rossi@ufrgs.br

Abstract. The search for mathematical and numerical models to address problems of nanostructures has gained centrality in the last two decades. This importance stems from the increasing applications of allotropic forms of carbon as nanotubes and more recently graphene in high-performance composite materials, resonators for high frequency, biosensors, gas sensors, among others. In fullerene nanotubes and graphene sheets, the natural frequencies are of the order of THz, a fact that enabled the application of these materials in ultra-frequency resonators and sensors based on the dispersion of mechanical waves in solid media. In the simulation of the dynamic behavior of nanostructures, the molecular dynamics (MD) method is frequently used, however, with a high computational cost. Recently, low-cost computational approaches based on the principles of non-local continuum mechanics have been used to include neighborhood effects of fundamental importance in the treatment of nanoscale problems. In this work, the authors propose the use of non-local continuous mechanics in the approach of free vibrations of axisymmetric nano-shells on Winkler's foundation modeled by first-order kinematic theories considering shear deformation (FSDT) and by cubic kinematic theories (TSDT). To increase the accuracy of the relatively high frequencies (above ten percent of the eigenvalues approximated by the numerical model) the approximation space will be built according to Uniform FEM B-Spline (U- FEM B-Spline) technique, with high order and high regularity. The results will be analyzed under three aspects: the sensitivity of the first natural frequency to variations in dimensions and the nanoscale coefficient; the relative error with respect to a target frequency; the relative error for a pre-stipulated frequency range.

Keywords: U-FEM B-Spline, FSDT, TSDT, shells.

1 Introduction

The simulation of the dynamic behavior of nanostructures has been the subject of recent research due to its importance in the study of super materials using allotropic forms of carbon. The use of nano structures of fullerene tubes (nano tubes) and graphene sheets (materials defined in 2D) has been widely researched in the last two decades due to the superior physical properties. In this context, it has been reported the high modulus of elasticity by Y. Nan and L. Vicenzo [1], the ability to detect high frequencies in the work of D. Garcia-Sanchez et al., [2], among others. On the other hand, in addressing the problem of free and forced vibrations on an atomic scale, classical or local solid mechanics was not shown adequate. In addressing dynamic problems on the atomic scale, the method of molecular mechanics (MM) and molecular dynamics (MD) has been widely used, as mentioned in the studies of: S.C. Chowdhury et al., [3] and [4], in the simulation of bonding forces in carbon chains and the problem of vibrations in graphene plates and by Belytschko et al. [5] in addressing the fracture problem in carbon nanotube chains, among others. This methodology, although very accurate, is computationally expensive using models with a small number of molecules involved to make computation possible. An alternative approach to the MD, but significantly less computationally expensive, is presented by Eringen [6] and [7] within the context of non-local continuum mechanics. In this theory the neighborhood effects on the atomic scale, extremely relevant in the constitutive equation, are considered. Recent work using this theory has been presented by S. Natarajan et al. [8] in addressing the problem of free vibrations in thin nano plates with a functional gradient using non-local

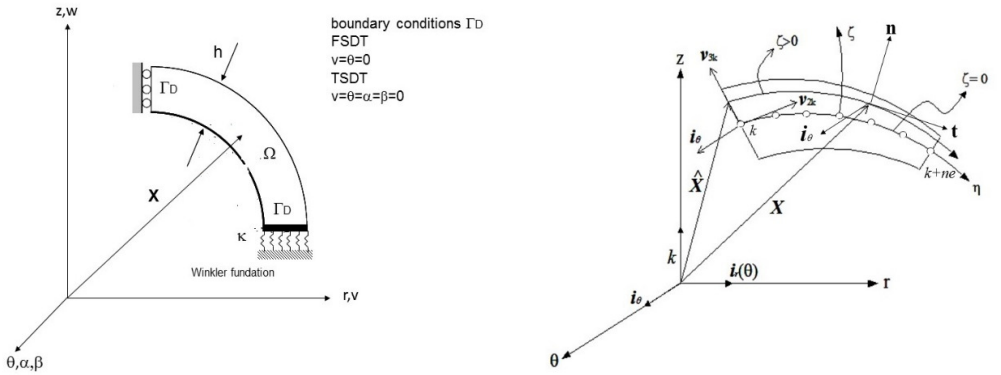
elasticity theory and the isogeometric method to obtain the approximation space; L. W. Zhang et al. [9] in the study of vibrations subjected to transverse magnetic field in thin square graphene nanoplates using an approximation space built according to the kp-Ritz element-free method; and other relevant studies that will not be mentioned in this document for brevity.

In the present work, the authors study the effect of variation in dimensions, of the nano-scale coefficients and regularity of approximation spaces on the axisymmetric natural modes and frequency of a hemispherical nano-shell over one Winkler's elastic foundation. The shell is modeled with a degenerated solid element described in cylindrical coordinates in J. L Bathoz and G. Dhatt [10], together with the first order shear deformation theory (FSDT) and the third shear deformation theory HSDT, both shown in J. N. Reddy [11]. The effect of the regularity of the approximation space on natural modes and frequencies is obtained using Uniform FEM B-Spline with C^2 and C^4 regularity, in the one-dimensional version, proposed by R. Burla [12]. The results are analyzed over three aspects: the sensitivity of the first natural frequency to the increment in dimensions and the nanoscale coefficient, the influence of the regularity of the approximation space on the convergence with respect to a relatively high target frequency (above ten percent of the numerically approximate modes) and the influence of the regularity of the approximation spaces in the decay of the first natural frequency with the increment of the nanoscale coefficients. This work is presented in five sections which are: introduction; discretized model of the free vibration problem using non-local elasticity; numerical results, conclusions, and bibliographic reference.

2 Free vibrations in non-local elasticity

In this section the problem of non-damped axisymmetric free vibrations is studied for a solid of revolution described in the plane of radial symmetry in Fig. 1 (a). The problem is to find the set of solutions $\{\boldsymbol{u}_i\}_{i=1}^{N}$ where $\boldsymbol{u}_i \in Kin$ (eq. (1)) satisfies the elliptical eigenvalues / eigenvectors problem described in non-local elasticity by equations (2) to (4) for the spectrum $0 \leq \omega_1 \leq \omega_2 \leq \cdots \omega_i \ldots \leq \omega_N$.

$$Kin = \left\{ \boldsymbol{u}(r,z) \neq \boldsymbol{0} \in C^2\left(\bar{\Omega}\right) \mid \boldsymbol{u}(r,z) = \boldsymbol{0},\ \boldsymbol{X}(r,z) \in \Gamma_D \right\} \tag{1}$$



(a) (b)

Figure 1: a) solid of revolution shown in the radial symmetry plane; b) degenerate solid element shown in cylindrical coordinates

$$\nabla \cdot \boldsymbol{\sigma}_l = -\omega^2 \rho \left(1 - \mu \nabla^2\right) \boldsymbol{u},\ \ \boldsymbol{X}(r,z) \in \Omega \tag{2}$$

$$\boldsymbol{\sigma}_l \cdot n = -\kappa \boldsymbol{u}, \qquad \boldsymbol{X}(r,z) \in \Gamma_D \tag{3}$$

$$\boldsymbol{u} = \boldsymbol{0},\ \boldsymbol{X}(r,z) \in \Gamma_D \tag{4}$$

In eq. (1) $\boldsymbol{\sigma}_l$ is the local stress tensor, ω the natural frequency, ρ the specific mass and μ the nanoscale coefficient. In eq. (2), κ is the spring stiffness that characterizes the Winkler foundation.

The weak discretized formulation is obtained for a shell of revolution modeled with a degenerated solid

element described in cylindrical coordinates (see Fib.1(b)) along with the FSDT and HSDT kinematic theories both described in J. N. Reddy [11]. The approximation space is obtained according to the Uniform FEM B-SPline methodology with regularity $C^k(\Omega)$ and polynomial order $p = k + 1,\ k = 2,4$, shown in R. Burla [12] and used in this work in the one-dimensional version. The Shape functions that approximate the displacement field are associated with the extreme nodes of the element shown in Fig.1 (b) and are described in detail in D. A. de Andrade et al. [13]. The description of the displacement field in the element according to the kinematic theories FSDT and HSDT is defined by eqs. (5) and (6) in global coordinates with sub-indexes f and t for the first and third order theories, respectively.

$$\boldsymbol{u}_{eh}\left(\eta,\zeta\right) = \begin{Bmatrix} v \\ w \end{Bmatrix}_{eh} = \boldsymbol{N}_f \boldsymbol{U}_f \tag{5}$$

$$\boldsymbol{u}_{eh}\left(\eta,\zeta\right) = \begin{Bmatrix} v \\ w \end{Bmatrix}_{eh} = \boldsymbol{N}_t \boldsymbol{U}_t \tag{6}$$

The explicit forms of the matrices in eqs. (5) and (6) are described by eqs. (7) to (10). In eq. (7) *ne* is the number of the last grid node of the element in Fig.1(b) and *nf* is the number of shape functions associated with the element's first and last node.

$$\boldsymbol{N}_f = \begin{bmatrix} \cdots & \phi_k^i\left(\eta\right) & 0 & \left(\phi_k^i\left(\eta\right) h_k \zeta \big/ 2\right) v_{2k}^r & \cdots \\ \cdots & 0 & \phi_k^i\left(\eta\right) & \left(\phi_k^i\left(\eta\right) h_k \zeta \big/ 2\right) v_{2k}^z & \cdots \end{bmatrix},\ k = 1, ne\ \ i = 1, nf \tag{7}$$

$$\boldsymbol{U}_f^T = \begin{Bmatrix} \cdots & v_k^i & w_k^i & \theta_k^i & \cdots \end{Bmatrix} \tag{8}$$

$$\boldsymbol{N}_t\left(\eta,\zeta\right) = \begin{bmatrix} \cdots & \phi_k^i & 0 & \left(\phi_k^i h_k \zeta \big/ 2\right) v_{2k}^r & \left(\phi_k^i h_k^2 \zeta^2 \big/ 4\right) v_{2k}^r & \left(\phi_k^i h_k^3 \zeta^3 \big/ 8\right) v_{2k}^r & \cdots \\ \cdots & 0 & \phi_k^i & \left(\phi_k^i h_k \zeta \big/ 2\right) v_{2k}^z & \left(\phi_k^i h_k^2 \zeta^2 \big/ 4\right) v_{2k}^z & \left(\phi_k^i h_k^3 \zeta^3 \big/ 8\right) v_{2k}^z & \cdots \end{bmatrix} \tag{9}$$

$$\boldsymbol{U}_t^T = \begin{Bmatrix} \cdots & v_k^i & w_k^i & \theta_k^i & \alpha_k^i & \beta_k^i & \cdots \end{Bmatrix} \tag{10}$$

In eqs. (7) to (10), $\phi_k^i\left(\eta\right)$ are B-Splines functions associated with the first and last node of the element, h_k is the thickness corresponding to the *k* node and $\boldsymbol{v}_{2k}^T = \left\{ v_{2k}^r, v_{2k}^z \right\}$ are the components of the tangent vector at node *k* to the Gaussian curve $\zeta = 0$.

The weak discretized formulation is obtained by the Galerkin method applied to the free vibration problem defined in equations (2) to (4) and resulting in the eq. (11).

$$\left[\sum_{e=1}^{n\Gamma_D} \int_{\Gamma_D} \kappa \boldsymbol{N}_e^T \boldsymbol{N}_e^m d\Gamma + \sum_{e=1}^{n\Gamma_D} \lambda \boldsymbol{N}_e^T \boldsymbol{N}_e^p d\Gamma + \sum_{e=1}^{n\Omega} \int_{\Omega_e} \boldsymbol{B}_e^T \boldsymbol{D} \boldsymbol{B}_e d\Omega \right] \boldsymbol{U}$$

$$-\omega^2 \left[\sum_{e=1}^{n\Omega} \left(\int_{\Omega_e} \rho \boldsymbol{N}_e^T \boldsymbol{N}_e d\Omega + \int_{\Omega_e} \mu\rho \boldsymbol{G}_e^T \boldsymbol{G}_e d\Omega \right) \right] \boldsymbol{U} = \boldsymbol{0} \tag{11}$$

In eq. (11), $\boldsymbol{U}$ is the vector of nodal displacement parameters that depends on the kinematic model used as mentioned in equations (8) and (10). Also, in eq. (11), λ is the penalty coefficient, $\boldsymbol{N_e}$, $\boldsymbol{B_e}$, and $\boldsymbol{D}$ are the kinematic, deformation and constitutive matrices described in detail for the FSDT and HSDT kinematic models in [13]. $\boldsymbol{N_e^p}$ and $\boldsymbol{N_e^m}$ are the penalty matrix of the essential boundary conditions and the matrix that represents the displacement component that produces spring deformation, both described for the FSDT model in eqs. (12) and (13).

$$\boldsymbol{N}_e^\alpha = \begin{bmatrix} \cdots & S_1^\alpha \phi_k^i\left(\eta\right) & 0 & S_3^\alpha \left(\phi_k^i\left(\eta\right) h_k \zeta \big/ 2\right) v_{2k}^r & \cdots \\ \cdots & 0 & S_2^\alpha \phi_k^i\left(\eta\right) & S_3^\alpha \left(\phi_k^i\left(\eta\right) h_k \zeta \big/ 2\right) v_{2k}^z & \cdots \end{bmatrix}. \tag{12}$$

$$S_j^{\alpha} = \begin{cases} 1, & j \; presc. \\ 0, j \; n \; / \; presc. \end{cases}; \; j = 1,...,3, \; \alpha = p, m. \tag{13}$$

Still in eq. (11) the matrices $\boldsymbol{G_e}$ defined in the eq. (14), is associated with the gradient $\nabla(.)$ operating in the displacement field.

$$\boldsymbol{G}_e = \boldsymbol{J}\partial_{\zeta}\boldsymbol{N}_e \tag{14}$$

In eq. (14) the operators ∂_{ζ} e $\boldsymbol{J}$ are shown in detail in O. A. G. de Suarez et al. [14]. Equation (11) is usually shown in matrix form in the problem of free vibrations by eq. (15).

$$\left[\boldsymbol{K} - \left(\boldsymbol{M}_l + \boldsymbol{M}_{nl}\right)\right]\boldsymbol{U} = \boldsymbol{0}. \tag{15}$$

In eq. (15), $\boldsymbol{K}$, $\boldsymbol{M}_l$ and $\boldsymbol{M}_{nl}$ represent the stiffness matrix, the local mass matrix and the non-local mass matrix all described explicitly in equations (16) to (18).

$$\boldsymbol{K} = \sum_{e=1}^{n\Gamma_D} \int_{\Gamma_D} \kappa \boldsymbol{N}_e^T \boldsymbol{N}_e^m d\Gamma + \sum_{e=1}^{n\Gamma_D} \lambda \boldsymbol{N}_e^T \boldsymbol{N}_e^p d\Gamma + \sum_{e=1}^{n\Omega} \int_{\Omega_e} \boldsymbol{B}_e^T \boldsymbol{D}\boldsymbol{B}_e d\Omega \tag{16}$$

$$\boldsymbol{M}_l = \sum_{e=1}^{n\Omega} \int_{\Omega_e} \rho \boldsymbol{N}_e^T \boldsymbol{N}_e d\Omega \tag{17}$$

$$\boldsymbol{M}_{nl} = \sum_{e=1}^{n\Omega} \int_{\Omega_e} \mu\rho \boldsymbol{G}_e^T \boldsymbol{G}_e d\Omega \, . \tag{18}$$

3 Numerical Result

The numerical results are obtained for the hemispherical shell on Winkler's elastic foundation with geometric characteristics and mechanical properties indicated in Fig. 1. In this section, the numerical results are analyzed from the perspective of the influence of the regularity of the approximation spaces on relatively high frequencies (ten percent above the frequencies obtained by the numerical model) and on the influence of the dimensions and coefficients of the nanoscale on the first resonant frequency. Still with a speculative character, the influence of the regularity of the approximation space on the decay of the first natural frequency is analyzed with the increase of the nanoscale coefficients.

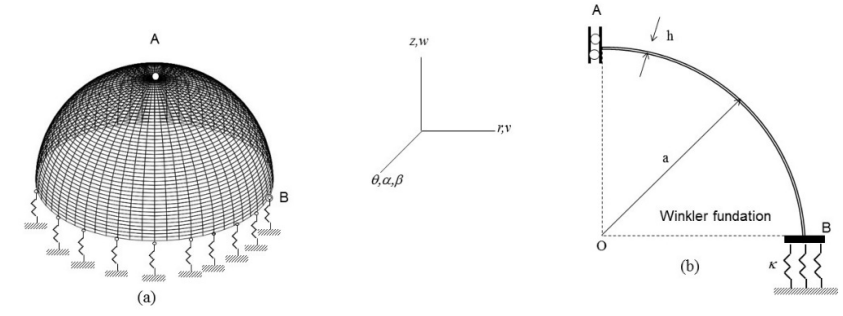


Figure 2: a) Hemispherical shell on Winkler foundation; b) boundary conditions in the symmetric radial plane.

3.1 Influence of approximation space regularity

The influence of approximation space regularity to obtain relatively high frequencies is analyzed for a hemispheric shell modeled with FSDT kinematic theory and with boundary conditions and mechanical and geometric properties indicated in case I of Fig. 2. In this study, the convergence analysis is performed by the relative error defined in eq. (19) for the target frequency ω_{60}. The approximation spaces are obtained by the "*h*" version presented in the strategies in the Tab.1. The reference solution ω_r in eq. (19) is obtained by the rule proposed in Dan Givoli [15] for an approximation space constructed with one hundred Lagrangian elements of six nodes (fifth polynomial order) resulting in a numerical model with 1498 degrees of freedom.

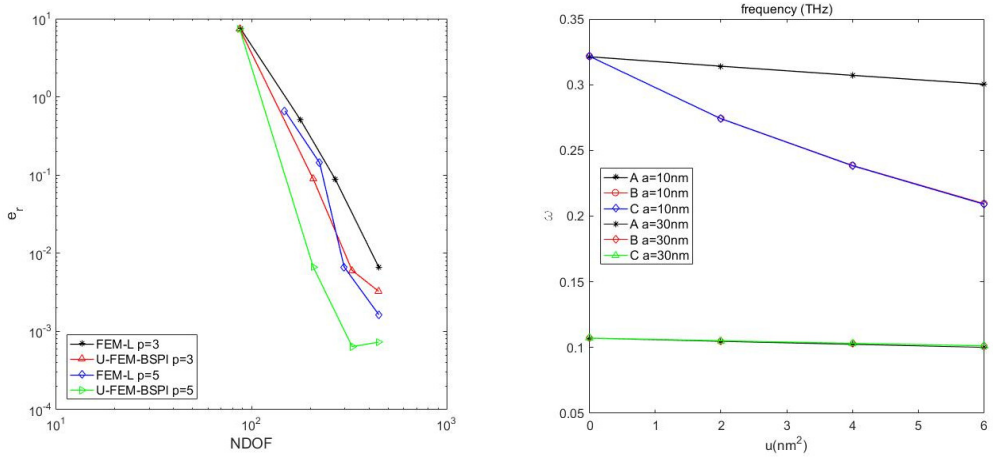
$$e_r = \left|\omega_h - \omega_r\right| \Big/ \left|\omega_r\right| \tag{19}$$

Table 1: Numerical strategies

FEM Lagrange				U-FEM B-Spline			
L_3		L_5		p=3		p=5	
nel.	NDOF	nel.	NDOF	grid	NDOF	grid	NDOF
10	88	10	148	29	87	29	87
20	178	15	223	69	207	69	207
30	268	20	298	109	327	109	327
50	448	30	448	149	447	149	447

In Tab.1, L^3 and L^5 are the one-dimensional Lagrangian elements of four nodes (cubic polynomial order) and the Lagrangian elements of six nodes (fifth polynomial order) respectively.

The results observed in the target frequency convergence studies in Fig.3 (a) show a significant improvement in the accuracy of the relatively high frequency obtained with approximation spaces build according to U-FEM B-Spline with respect to those obtained with FEM Lagrange. This fact, already mentioned in T. J. R. Hughes [16] and [15], is due to the regularity C^2 and C^4 of the approximation spaces built according to Uniform FEM B-SPline.



(a) (b)

Figure 3: a) convergence to target frequency ω_{60}; b) influence of dimensions and nano scale coefficient in first resonant frequency.

3.2 Influence of dimensions and nanoscale coefficients on the first natural frequency

The influence of the variation of the nanoscale coefficient and of the dimensions in the first natural frequency is analyzed for the shell indicated in Fig.1 with geometric and mechanical properties shown in case II. This study

considered the increase in nanoscale coefficients $\mu = \{0,2,4,6\}(nm^2)$ and the dimensions $a = \{10,30\}(nm)$. The numerical models used are described in items A, B and C in Tab.2. The results of this study are shown in Fig.3 (b).

Table 2: proposed strategies

A			B			C		
FEM C^0		FSDT	U-FEM B-SPline C^2		FSDT	U-FEM B-SPline C^2		HSDT
elem.	eltype	NDOF	grid	p	NDOF	grid	p	NDOF
50	L3	448	149	3	447	149	3	745

From the analysis of Fig. 3, an evident fact emerges that is based on the theory of non-local elasticity of Eringen [7]. With the increase of the dimensions of the structure the results for different values of nanoscale coefficients converge to that obtained by the classical elasticity with $\mu = 0$. Another aspect of the analysis refers to the significant difference in the decay of the first natural frequency observed in Fig. 3 (b) of strategy A in relation to strategies B and C for the shell with a = 10nm. A speculation about the greater sensitivity to behavior on the nanoscale, shown by the strategies that build the approximation spaces using U-FEM B-SPline, is in the fact that it presents continuity in the solution gradient that directly affects the non-local mass matrix as it is shown in eq. (11).

4 Conclusions

The effects of the regularity of the approximation spaces in the numerical approach to the eigenvalue / eigenvector problem (version of the free vibration problem) qualitatively confirm the results obtained in M. Rauen et al. [17], J. A. Cottrell et al. [18] and [19], in the analysis of free vibrations of a hemispheric nano-shell within the limits of classical elasticity, that is, with $\mu = 0$. The sensitivity on the first natural frequency of the nanoscale coefficients and shell dimensions was found according to Eringen's theory [7]. Another aspect found in the analysis of this work is related to the influence of the regularity of the approximation space on the decay of the frequency values with the increase of the nanoscale coefficients. This fact is possibly due to the use of the gradient of the approximation solutions in obtaining the non-local mass matrix. In this case, the approach spaces built with regularity C^2 and C^4 guarantee the continuity of the gradient, which does not happen with the approach spaces built according to the FEM C^0.

Acknowledgements. The authors of this work would like to thank CAPES for financial support through the postdoctoral scholarship and the infrastructure provided by UFRGS. Also, to the CNPq and FAPERGS for financial research support. Grant numbers: CNPq 306058/2018-9, FAPERGS: 19/2551-0001954-8-1.

Authorship statement. The authors confirm that they are solely responsible for the authorship of this work, and that all material that has been included here as part of this paper is either owned (and authored) by the authors or has the permission of the owners to be included here.

References

[1] Nao Y. and Vicenzo L. "Young's Modulus of single walled carbon nanotube". *Journal of Applied Phisics*, vol. 84, n. 4, 1998.
[2] D. Garcia-Sanchez, A. San Paulo, M. J. Esplandiu, F. Perez-Murano, L. Forro´, A. Aguasca, and A. Bachtold. "Mechanical detection of carbon nanotube resonator vibration". *Phisical Review Letters*, vol. 99, n. 085501, 2007.
[3] S.C. Chowdhury, T. Okabe. "Computer simulation of carbon nanotube pull-out from polymer by the molecular dynamics method". *Composites: Part A,* vol. 38, pp 747–754, 2007.
[4] R Chowdhury, S Adhikari1, F Scarpa and M I Friswell. "Transverse vibration of single-Layer graphene Sheets". *Journal of physics D: Applied Physics*, vol 44, 205401 (11pp), 2011.
[5] T. Belytschko, S. P. Xiao, G. C. Schatz, and R. S. Ruoff. "Atomistic simulations of nanotube fracture". *Physical review B*, vol. 65, 235430, 2002.

[6] A. C. Eringen. "Theory of micromorphic materials of with memory". *International Journal of Engineering and Science*, vol. 10, pp 623-641, 1972.
[7] A. C. Eringen. "On differential equations of nonlocal elasticity and solutions of screw dislocation and surface waves". *Journal of Applied Physic*, vol. 54, n. 4703, 1983.
[8] S. Natarajan, S. Chakraborty, M. Thangavel, S. Bordas, T. Rabczuk. "Size-dependent free flexural vibration behavior of functionally graded nanoplates". *Computational Materials Science,* vol. 65 pp 74–80, 2012.
[9] L.W. Zhang, Yang Zhang, K.M. Liew. "Vibration analysis of quadrilateral graphene sheets subjected to an inplane magnetic field based on nonlocal elasticity theory". *Composites Part B*, vol. 118, pp 96-103, 2017.
[10] J. L. Batoz, G. Dhatt. *Modélisation des structures par élements finis*. Hermès, Paris, 1992.
[11] J. N. Reddy. *Mechanics of laminated composite plates and shells theory and analysis*. CRC Press LLC, 2004.
[12] R. C. Burla. Finite Element Analysis using Uniform B-Spline approximation and implicit boundary method. Phd Thesis of Florida University, 2008.
[13] D. A. de Andrade, A. F. Michels, O. A. Garcia. "Uniform FEM B-Spline na abordagem de problemas de vibrações livres e forçadas em cascas laminadas". *XXXVIII Iberian Latin-American Congress on Computational Methods in Engineering,* ABMEC, Florianópolis, SC, Brazil, November 2017.
[14] O. A. G. de Suarez, R. Rossi, C. R. A. da Silva Jr. "Enrichment of rational polynomial family of shape functions with regularity $C_0^k, k = 0,2,4,..$ Applications in axisymmetric plates and shells". Engineering Computations, vol. 29, pp 636-660, 2012.
[15] Dan Givoli. "On the number of reliable finite-element eigenmodes". *Communications in numerical methods in engineering*, vol. 24, pp 1967–1977, 2008.
[16] T. J. R. Hughes. The Finite Element Method Linear Static and Dynamic Finite Element Analysis. Englewood Cliffs, N. J.: Prentice-Hall, 1987.
[17] M. Rauen, R. D. Machado, M. Arndt. "Isogeometric Analysis Applied to Free Vibration Analysis of Plane Stress and Plane Strain Structures". *XXXVII Iberian Latin American Congress on Computational Methods in Engineering*, Brasilia, Brasil, 2016.
[18] J.A. Cottrell, A. Reali, Y. Bazilevs, T.J.R. Hughes. "Isogeometric analysis of structural vibrations". *Computer Methodos in Applied Mechanics and Engineering*, vol.195, pp5257-5296, 2006.
[19] J. A. Cottrell, T. J. R. Hughes, A. Reali. "Studies of refinament and continuity in isogeometric structural analysis", *Computer Methods in Applied Mechanics and Engineering*, vol.196, pp4160-4183, 2007.