Vibration Analysis of Carbon Nanotubes Using the Spline Collocation Method

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Abstract: This work investigates carbon nanotube frequencies via continuum mechanics based spline collocation approach simulations using nanobeam-bending models. The spline collocation formulas are verified by comparing numerical results to analytic and experimental results published in the literature. It is shown that the spline collocation method simulation results are in good agreement with the experimental data from literatures. The current modeling approach is suitable for the development of carbon nanotube applications.

Keywords: spline collocation method, carbon nanotube, vibration analysis, nanomechanical behavior, nature frequency, finite element method

INTRODUCTION

Carbon nanotubes have good nanomechanical and electrical characteristics. Nanotechnology has become one of the critical technologies of this century. Wang et al. (2001), (H. Rafii-Tabar, 2004) modeled and measured experimentally strengths of nanotubes in bending and compression. The finite element analysis has been used for rapid computation of the nanomechanical behavior of carbon nanotubes (D. H. Wu, et al., 2006; K. T. Lau, et al., 2004). Ke et al. 2005, N. Pugno, et al., (2005), studied singly and doubly clamped nanotubes under electrostatic actuation. Keblinski et al. (P. Keblinski, 2002; K. A. Bulashevich, and S. V. Rotkin, 2002) observed essentially classical distribution of charge density with a significant charge concentration at the tube end of conductive nanotubes. Poncharal et al. (1999) presented that static and dynamic mechanical deflections were electrically induced in cantilevered, multiwalled carbon nanotubes in a transmission electron microscope. The nanotubes were resonantly excited at the fundamental frequency and high harmonics as revealed by their deflected contours, which correspond closely to those determined for cantilevered elastic beams (Poncharal et al. 1999). The spline collocation method is employed to formulate the electrostatic field problems in a matrix form in this work. The integrity and computational accuracy of the spline collocation method in solving this problem will be evaluated through a range of case studies.

Bending Vibration of Carbon Nanotubes:

Figure 1 shows the geometry and boundary conditions for the carbon nanotube. Based on the Euler-Bernoulli beam model, the corresponding kinetic energy of the carbon nanotube is

\[ T = \frac{1}{2} \rho A \left( \frac{\partial \psi(x,t)}{\partial t} \right)^2 dx \]  

where \( \psi \) is displacement, \( t \) is time, \( A \) is area of nanotube cross section, \( \rho \) is density of nanotube material. The strain energy of the carbon nanotube can be found as

\[ U = \frac{1}{2} E I \left( \frac{\partial^2 \psi(x,t)}{\partial x^2} \right)^2 dx \]
where \( I \) is the second moment of cross-sectional area \( A \), 
\[
I = \left( \pi \left( \frac{D_{\text{out}}}{2} \right)^4 - \left( \frac{D_{\text{in}}}{2} \right)^4 \right) / 4
\]
is Young's modulus of the carbon nanotube material. The Hamilton's principle is

\[
\int_{\dot{q}} \left( \delta T - \delta U + \delta W \right) \, dx = 0
\]

where \( \delta W \) is the virtual work. Substituting Eqs. (1) and (2) into Eq. (3) yields the equations of motion for the carbon nanotube. The transverse motion \( w(x,t) \) of a carbon nanotube is governed by

\[
\frac{\partial^2}{\partial x^2} \left( EI \frac{\partial^2 w}{\partial x^2} \right) + \rho A \frac{\partial^2 w}{\partial t^2} = 0
\]

Consider the carbon nanotube to be clamped at the end \( x = 0 \), the corresponding boundary conditions are

\[
w(0,t) = 0
\]

\[
\frac{\partial w(0,t)}{\partial x} = 0
\]

\[
EI \frac{\partial^2 w(L,t)}{\partial x^2} = 0
\]

\[
\frac{\partial}{\partial x} \left( EI \frac{\partial^2 w(L,t)}{\partial x^2} \right) = 0
\]

In order to obtain the frequencies, a harmonic movement of the carbon nanotube is assumed as follows:
where \( W(x) \) is the vibration mode, \( \omega \) is the natural frequency of carbon nanotube. Substituting Eq. (9) into Eq. (4), leads to

\[
\frac{d^2 EI}{dx^2} \frac{d^2 W}{dx^2} + 2 \frac{d EI}{dx} \frac{d^3 W}{dx^3} + EI \frac{d^4 W}{dx^4} = \omega^2 \rho A W
\]  

(10)

The fixed-fixed boundary conditions are

\[
W(0) = 0
\]  

(11)

\[
\frac{dW(0)}{dx} = 0
\]  

(12)

\[
W(L) = 0
\]  

(13)

\[
\frac{dW(L)}{dx} = 0
\]  

(14)

The simple-supported boundary conditions are

\[
W(0) = 0
\]  

(15)

\[
EI \frac{d^2 W(0)}{dx^2} = 0
\]  

(16)

\[
W(L) = 0
\]  

(17)

\[
EI \frac{d^2 W(L)}{dx^2} = 0
\]  

(18)

The clamped-free boundary conditions are

\[
W(0) = 0
\]  

(19)

\[
\frac{dW(0)}{dx} = 0
\]  

(20)

\[
EI \frac{d^2 W(L)}{dx^2} = 0
\]  

(21)

\[
\frac{d}{dx} \left( EI \frac{d^2 W(L)}{dx^2} \right) = 0
\]  

(22)

**Finite Element Method Modeling:**

In order to derive finite formulations, the following virtual work principle must be utilized (J.N. Reddy, 1993; K.J. Bathe, 1982):
where $[\varepsilon]$ is a strain matrix, $[\sigma]$ is a stress matrix, $[w']$ is a displacement matrix, and $[f]$ is a inertia force matrix. The stress-strain relation for linear conditions reads:

$$[\sigma] = [D][\varepsilon]$$

where $[D]$ is an elastic matrix. The finite element method can convert any differential equation to a set of algebraic equations. It assumes the shape of solution in the domain of element and satisfies equilibrium. A finite element solution is assumed as (J.N. Reddy, 1993; K.J. Bathe, 1982)

$$w^* = [N][w^*] \cos(\alpha t)$$

where $[N]$ is the matrix of any suitable assumed shape function. The tetrahedral mesh is used in this model. The finite element assembles all elements to form a complete structure to equilibrate the structure with its environment. The equation of the finite element model for the carbon nanotube is

$$[K^*][w^*] = \omega^2 [M^*][w^*]$$

where $[M^*]$ is the mass matrix and $[K^*]$ is the stiffness matrix. The mass matrix can be written as

$$[M^*] = \int [B]^T[D][B]dV$$

where $[L]$ is a linear differential operator matrix. The stiffness matrix can be written as

$$[K^*] = \int [B]^T[D][B]dV$$

The order of the matrix is $N \times N$. $N$ is the number of nodes at which the solution is not known. A nontrivial solution to Eq. (26) exists only if the determinant of the coefficient matrix is zero:

$$[K^*] - \omega^2 [M^*] = 0$$

The eigenvalues of the carbon nanotube can be determined from Eq. (30). The convergence and accuracy of the finite element solution depends on the differential equation, integral form, and elements used. The computational solution is obtained by the finite element method, which is widely applied in engineering design.

**The Spline Collocation Method Modeling:**

The solutions to numerous complex nanobeam problems have been efficiently obtained as the use of fast computers and the range of available numerical methods, including the Galerkin method, finite element technique, boundary element method, and Rayleigh-Ritz method. In this study, spline collocation method is employed to formulate the discrete eigenvalue problems of various carbon nanotubes. Prenter et al. (1969.)

\[ x_i = a + ih \text{ for } i = -2, -1, 0, \ldots, N + 1, N + 2 \]  
\[ h = \frac{b - a}{N} \]  
\[ B(x) = \begin{cases}  
\frac{(x - x_{i-2})}{h}, & x \in [x_{i-2}, x_{i-1}] \\
\frac{(x - x_{i-2}) - 6(x - x_{i-1})}{h}, & x \in [x_{i-1}, x_i] \\
\frac{(x - x_{i-2}) - 6(x - x_{i-1}) + 15(x - x_{i-2})}{h}, & x \in [x_{i-1}, x_i] \\
\frac{(x - x_{i-2}) - 6(x - x_{i-1}) + 15(x - x_{i-2}) - 20(x - x_i)}{h}, & x \in [x_{i-2}, x_{i+1}] \\
\frac{(x - x_{i-2}) - 6(x - x_{i-1}) + 15(x - x_{i-2}) - 20(x - x_i) + 15(x - x_{i-3})}{h}, & x \in [x_{i-2}, x_{i+1}] \\
\frac{(x - x_{i-2}) - 6(x - x_{i-1}) + 15(x - x_{i-2}) - 20(x - x_i) + 15(x - x_{i-3}) - 6(x - x_{i-4})}{h}, & x \in [x_{i-1}, x_{i+1}] \\
0, & \text{otherwise} 
\end{cases} \]

where $B_{-2}(x), B_{-1}(x), B_0(x), \ldots, B_{N+1}(x), B_{N+2}(x)$ form the region $a \leq x \leq b$. Spline function is given as follows (P. M. Prenter, 1969; C. W. Bert, and Y. Sheu, 1996).

For a function $W(x)$ is given by the following equation.

\[ W(x) = \sum_{i=2}^{N+2} a_i B_i(x) \]  

where $a_i$ is constant, and $B_i(x)$ is the spline function. There are $N+5$ collocation points in the domain. The equation of motion of a carbon nanotube can be rearranged into the spline collocation method formula by substituting Eq. (35) into Eq. (4). This leads to

\[ \begin{bmatrix} \frac{d^2 EI(x_i)}{dx^2} & \frac{d^2 B_{N+2}(x_i)}{dx^2} & \frac{d^2 EI(x_i)}{dx^2} & \frac{d^2 B_{N+1}(x_i)}{dx^2} & \frac{d^2 EI(x_i)}{dx^2} & \frac{d^2 B_N(x_i)}{dx^2} & \cdots \\
\frac{d^2 EI(x_i)}{dx^2} & \frac{d^2 B_{N+2}(x_i)}{dx^2} & \frac{d^2 EI(x_i)}{dx^2} & \frac{d^2 B_{N+1}(x_i)}{dx^2} & \frac{d^2 EI(x_i)}{dx^2} & \frac{d^2 B_N(x_i)}{dx^2} \end{bmatrix} \begin{bmatrix} a_{j1} \\
\vdots \\
A_{jN} \end{bmatrix} = \begin{bmatrix} p_{j1} \\
p_{j2} \\
p_{jN} \end{bmatrix} \]
Using the spline collocation method, the boundary conditions of a clamped-clamped carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
2 \frac{dEI(x_i) d^3 B_{-2}(x_i)}{dx^3} & 2 \frac{dEI(x_i) d^3 B_{-1}(x_i)}{dx^3} & 2 \frac{dEI(x_i) d^3 B_{0}(x_i)}{dx^3} & \cdots \\
2 \frac{dEI(x_i) d^3 B_{N+1}(x_i)}{dx^3} & 2 \frac{dEI(x_i) d^3 B_{N+2}(x_i)}{dx^3} \\
\end{bmatrix} \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} + \\
\begin{bmatrix}
EI(x_i) \frac{d^4 B_{-2}(x_i)}{dx^4} & EI(x_i) \frac{d^4 B_{-1}(x_i)}{dx^4} & EI(x_i) \frac{d^4 B_{0}(x_i)}{dx^4} & \cdots \\
EI(x_i) \frac{d^4 B_{N+1}(x_i)}{dx^4} & EI(x_i) \frac{d^4 B_{N+2}(x_i)}{dx^4} \\
\end{bmatrix} \begin{bmatrix} a_{j2} \\ \vdots \end{bmatrix} = 0
\]  

Using the spline collocation method, the boundary conditions of a simple-supported carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
\omega^2 \rho A(x_i) B_{-2}(x_i) & \omega^2 \rho A(x_i) B_{-1}(x_i) & \omega^2 \rho A(x_i) B_{0}(x_i) & \cdots \\
\omega^2 \rho A(x_i) B_{N+1}(x_i) & \omega^2 \rho A(x_i) B_{N+2}(x_i) \\
\end{bmatrix} \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} = 0
\]  

for \( i = 0, 1, \ldots, N \) and \( j = -2, -1, \ldots, N + 2 \)

Using the spline collocation method, the boundary conditions of a clamped-clamped carbon nanotube can be rearranged into the matrix form as

\[
[ B_{-2}(x_0) \quad B_{-1}(x_0) \quad B_0(x_0) \quad \cdots \quad B_{N+1}(x_0) \quad B_{N+2}(x_0) ] \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} = 0
\]  

for \( j = -2, -1, \ldots, N + 2 \)

Using the spline collocation method, the boundary conditions of a simple-supported carbon nanotube can be rearranged into the matrix form as

\[
[ B_{-2}(x_0) \quad B_{-1}(x_0) \quad B_0(x_0) \quad \cdots \quad B_{N+1}(x_0) \quad B_{N+2}(x_0) ] \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} = 0
\]  

for \( j = -2, -1, \ldots, N + 2 \)

Using the spline collocation method, the boundary conditions of a simple-supported carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
\frac{dB_{-2}(x_0)}{dx} & \frac{dB_{-1}(x_0)}{dx} & \frac{dB_0(x_0)}{dx} & \cdots & \frac{dB_{N+1}(x_0)}{dx} & \frac{dB_{N+2}(x_0)}{dx} \\
\frac{dB_{-2}(x_0)}{dx} & \frac{dB_{-1}(x_0)}{dx} & \frac{dB_0(x_0)}{dx} & \cdots & \frac{dB_{N+1}(x_0)}{dx} & \frac{dB_{N+2}(x_0)}{dx} \\
\end{bmatrix} \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} = 0
\]  

for \( j = -2, -1, \ldots, N + 2 \)

Using the spline collocation method, the boundary conditions of a simple-supported carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
\frac{dB_{-2}(x_0)}{dx} & \frac{dB_{-1}(x_0)}{dx} & \frac{dB_0(x_0)}{dx} & \cdots & \frac{dB_{N+1}(x_0)}{dx} & \frac{dB_{N+2}(x_0)}{dx} \\
\frac{dB_{-2}(x_0)}{dx} & \frac{dB_{-1}(x_0)}{dx} & \frac{dB_0(x_0)}{dx} & \cdots & \frac{dB_{N+1}(x_0)}{dx} & \frac{dB_{N+2}(x_0)}{dx} \\
\end{bmatrix} \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} = 0
\]  

for \( j = -2, -1, \ldots, N + 2 \)

Using the spline collocation method, the boundary conditions of a simple-supported carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
\frac{dB_{-2}(x_N)}{dx} & \frac{dB_{-1}(x_N)}{dx} & \frac{dB_0(x_N)}{dx} & \cdots & \frac{dB_{N+1}(x_N)}{dx} & \frac{dB_{N+2}(x_N)}{dx} \\
\frac{dB_{-2}(x_N)}{dx} & \frac{dB_{-1}(x_N)}{dx} & \frac{dB_0(x_N)}{dx} & \cdots & \frac{dB_{N+1}(x_N)}{dx} & \frac{dB_{N+2}(x_N)}{dx} \\
\end{bmatrix} \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} = 0
\]  

for \( j = -2, -1, \ldots, N + 2 \)

Using the spline collocation method, the boundary conditions of a simple-supported carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
\frac{dB_{-2}(x_0)}{dx} & \frac{dB_{-1}(x_0)}{dx} & \frac{dB_0(x_0)}{dx} & \cdots & \frac{dB_{N+1}(x_0)}{dx} & \frac{dB_{N+2}(x_0)}{dx} \\
\frac{dB_{-2}(x_0)}{dx} & \frac{dB_{-1}(x_0)}{dx} & \frac{dB_0(x_0)}{dx} & \cdots & \frac{dB_{N+1}(x_0)}{dx} & \frac{dB_{N+2}(x_0)}{dx} \\
\end{bmatrix} \begin{bmatrix} a_{j1} \\ \vdots \end{bmatrix} = 0
\]  

for \( j = -2, -1, \ldots, N + 2 \)
Using the spline collocation method, the boundary conditions of a clamped-free carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
EI(x_0) \frac{d^2 B_2(x_0)}{dx^2} & EI(x_0) \frac{d^2 B_1(x_0)}{dx^2} & EI(x_0) \frac{d^2 B_0(x_0)}{dx^2} \\
\vdots & \vdots & \vdots \\
EI(x_N) \frac{d^2 B_{N+1}(x_N)}{dx^2} & EI(x_N) \frac{d^2 B_{N+2}(x_N)}{dx^2} & \{a_j\} = 0
\end{bmatrix}
\]

for \( j = -2, -1, \cdots, N + 2 \)

\[
\begin{bmatrix}
B_2(x_N) & B_1(x_N) & B_0(x_N) \\
\vdots & \vdots & \vdots \\
B_{N+1}(x_N) & B_{N+2}(x_N) & \{a_j\} = 0
\end{bmatrix}
\]

for \( j = -2, -1, \cdots, N + 2 \)

Using the spline collocation method, the boundary conditions of a clamped-free carbon nanotube can be rearranged into the matrix form as

\[
\begin{bmatrix}
B_2(x_0) & B_1(x_0) & B_0(x_0) \\
\vdots & \vdots & \vdots \\
B_{N+1}(x_N) & B_{N+2}(x_N) & \{a_j\} = 0
\end{bmatrix}
\]

for \( j = -2, -1, \cdots, N + 2 \)

\[
\begin{bmatrix}
\frac{dB_2}{dx}(x_0) & \frac{dB_1}{dx}(x_0) & \frac{dB_0}{dx}(x_0) \\
\vdots & \vdots & \vdots \\
\frac{dB_{N+1}}{dx}(x_N) & \frac{dB_{N+2}}{dx}(x_N) & \{a_j\} = 0
\end{bmatrix}
\]

for \( j = -2, -1, \cdots, N + 2 \)

\[
\begin{bmatrix}
EI(x_N) \frac{d^2 B_2(x_N)}{dx^2} & EI(x_N) \frac{d^2 B_1(x_N)}{dx^2} & EI(x_N) \frac{d^2 B_0(x_N)}{dx^2} \\
\vdots & \vdots & \vdots \\
EI(x_N) \frac{d^2 B_{N+1}(x_N)}{dx^2} & EI(x_N) \frac{d^2 B_{N+2}(x_N)}{dx^2} & \{a_j\} = 0
\end{bmatrix}
\]

for \( j = -2, -1, \cdots, N + 2 \)

\[
\begin{bmatrix}
EI(x_N) \frac{d^3 B_2(x_N)}{dx^3} & EI(x_N) \frac{d^3 B_1(x_N)}{dx^3} & EI(x_N) \frac{d^3 B_0(x_N)}{dx^3} \\
\vdots & \vdots & \vdots \\
EI(x_N) \frac{d^3 B_{N+1}(x_N)}{dx^3} & EI(x_N) \frac{d^3 B_{N+2}(x_N)}{dx^3} & \{a_j\} = 0
\end{bmatrix}
\]

for \( j = -2, -1, \cdots, N + 2 \)
The obtained results are summarized in the following figures.

RESULTS AND DISCUSSION

Results:

Figure 2 shows the calculated frequencies of the fixed–fixed carbon nanotube solved using the spline collocation method. The material and geometric parameters of the nanotube are $D_{\text{ext}} = 33$ nanometer, $D_{\text{int}} = 18.8$ nanometer, $L = 5.5$ micrometer, $\rho = 2.2 \times 10^3$ kg/m$^3$, and $E = 32$ GPa. Frequency is defined as $f = \omega / 2\pi$. Computational results are compared successfully with those obtained by the spline collocation method and finite element method results. Figure 3 plots the frequencies of the simple supported carbon nanotube. The difference is defined as

$$\text{Difference}(\%) = \left( \frac{f - f_{\text{exp}}}{f_{\text{exp}}} \right) \times 100(\%)$$

Fig. 2: Frequencies of the fixed-fixed carbon nanotube.
Fig. 3: Frequencies of the simple supported carbon nanotube.

Fig. 4: Frequencies of the fixed-free carbon nanotube.

The first experimental frequency is $0.658\text{MHz}$ (Z. L. Wang, et al., 2001). The discrepancy between the numerical results and the experimental data (Z. L. Wang, et al., 2001) is 180%. Numerical results imply that the frequencies calculated from the proposed spline collocation method are very consistent with the experimental results published in the literature (Z. L. Wang, et al., 2001). It may be observed from this figure the curve solved using the spline collocation method closely follows the curve solved using the finite element method. Figure 5 displays the frequencies of the fixed-free carbon nanotube. The material and geometric
Fig. 5: Frequencies of the fixed-free carbon nanotube.

parameters of the carbon nanotube are as follows: \( D_{\text{out}} = 39 \) nanometer \( D_{\text{in}} = 19.4 \) nanometer \( L = 5.7 \) micron \( \rho = 2.2 \times 10^3 \) kg/m\(^3\) \( E = 26.5 \) GPa and 0.644 MHz (Z.L. Wang, et al., 2001). The difference between the numerical results and the experimental data (Z.L. Wang, et al., 2001) is 107%. The agreement between numerical and experimental results and is satisfactory.  Figure 6 shows the frequencies of the fixed-free carbon nanotube. The material and geometric parameters of the carbon nanotube are given as: \( D_{\text{out}} = 39 \) nanometer \( D_{\text{in}} = 13.8 \) nanometer \( L = 5 \) micron \( \rho = 2.2 \times 10^3 \) kg/m\(^3\) \( E = 26.3 \) GPa and
Fig. 7: Frequencies of the fixed-free carbon nanotube.

Fig. 8: Frequencies of the fixed-free carbon nanotube.

MHz (Z.L. Wang, et al., 2001). The discrepancy between the numerical results and the experimental data (Z. L. Wang, et al., 2001) is 1.18%. Computational results indicate that the frequencies calculated using the spline collocation and finite element methods agreed very well with the measured frequencies. Figure 7 reveals the frequencies of the carbon nanotube. The material and geometric parameters of the fixed-free carbon nanotube are $D_{nw}=45.8$ nanometer, $D_{n}=16.7$ nanometer, $L=5.3$ micrometer, $\rho=2.2 \times 10^3$ kg/m$^3$, $E=31.5$ GPa. The first experimental frequency is (Z.L. Wang, et al., 2001). The difference between the numerical results and the experimental data (Z.L. Wang, et al., 2001) is 1.17%. The numerical results and the results measured experimentally correspond closely. Figure 8 points the frequencies of the carbon nanotube. The material and geometric parameters of the
Fig. 9: Frequencies of the fixed-free carbon nanotube.

The first experimental frequency is 1.14%. The agreement between numerical and experimental results is good enough. Figure 9 lists the frequencies of the fixed-free carbon nanotube. The material and the geometric parameters of the carbon nanotube are

\[ \rho = 2.2 \times 10^3 \text{ kg/m}^3 \quad E = 321 \text{ GPa} \quad \text{and} \]

The first experimental frequency is 0.35%. Computational results imply that the frequencies calculated from the proposed spline collocation method and the finite element method are highly consistent with the experimental results published in the literature (Z.L. Wang, et al., 2001). The spline collocation method is a more accurate numerical method with same versatility and efficient as the finite element method by comparison between the finite element method and the spline collocation approach.

**Conclusions:**

The spline collocation method is successfully applied to analyze the nanomechanical characteristics of carbon nanotubes. Experimental frequencies published in the literature are extremely consistent with the frequencies determined using the spline collocation method. This study has developed that the continuum mechanics method is combined with the spline collocation method to simulate the vibration properties of the carbon nanotubes. The study demonstrates the value of the spline collocation method for the dynamic behavior of carbon nanotubes.

**REFERENCES**


