# Numerical Analysis of Nanowire Resonators for Ultra-high Resolution Mass Sensing in Biomedical Applications

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# Numerical Analysis of Nanowire Resonators for Ultra-high Resolution Mass Sensing in Biomedical Applications



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**Abstract** Nanowire resonators have fascinated researchers as a promising group of devices for accurate detection of tiny objects such as atoms, molecules, viruses, bacteria, and different types of bio-objects. In this paper, we present a numerical solution to the newly developed mathematical model of the nanowire resonator, considering such important characteristics as temperature variations, as well as the electromagnetic fields, added mass, surface and nonlocal effects. The mathematical model is based on the nonlocal Euler-Bernoulli beam theory. The developed model is solved by using the Finite Difference Method (FDM). As a result of this solution, the frequency response of the nanowire resonator has been obtained. Then, based on the developed numerical solution, a parametric study has been carried out to investigate the effects of different parameters on the vibration of nanowire resonators. Finally, the importance of nonlinearity in the modelling of such resonators at the nanoscale has been highlighted.

**Keywords** ■■■

## 1 Introduction

The extraordinary and unique mechanical properties of nanostructures have made them an excellent candidate for mass sensing applications. Different types of nanoresonators including nanowires, quantum dots, nanotubes and graphene sheets have been studied by researchers from different fields to be used for tiny object detec- AQ1

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tion. In particular, the ultra-high frequency of these structures attracted attention of researchers in the area of bio-sensing to implement them for the detection of tiny bio-objects. As a result, plenty of theoretical and practical approaches have been proposed for the detection of tiny bio-particles. By using both theoretical and experimental approaches, researchers have shown a strong potential of nanoresonators in the detection of tiny objects even in the scale of zeptogram (zg) [1–3].

Nanoresonators, specifically semi-conducting nanowires, have shown very unique reproducible and tunable conducting properties, which provide a basis for strong sensing approaches in medical applications [4]. This high resolution of sensing allows detection of tiny bio-objects such as DNA, RNA, proteins, viruses, bacteria and very small chemical atoms. Analysis of temperature variations is one of the well-addressed parameters, but in order to analyze other significant parameters, the development of novel models is needed to provide a better understanding of nanoresonator's sensing resolution. Thus, vibration characterization and parametric sensitivity analysis of nano-mechanical resonators for sensing applications are crucial, notably in biomedicine. It should be noted that when we refer to nanosensors, we deal with a resonator with dimensions in the order of nanometer, which has sensitivity in the nanoscale range, and its interaction distance with the object being detected in nanometer size. That is why a small perturbation with different sources of excitation such as temperature, electromagnetic field, nonlinearity due to large oscillations of the nanoresonators or their substrates should be taken into account for an adequate mathematical modelling of these devices. Accordingly, vibrations of nanoresonators including nanobeams, quantum dots, nanotubes, nanowires, graphene sheets, and nanoplates have been receiving an increased attention in the interdisciplinary community of researchers, including those working in the areas of applied mechanics and mathematics, structural analysis and vibrations. A number of works have been published so far to investigate the vibrations of nanoresonators [5–8].

An analysis of the state-of-the-art in this field shows that there is a lack of modelling results for nanowire resonators in mass detection applications that take into account different critical parameters such as the electromagnetic fields, piezoelectric potential, nonlinearity, external excitations and thermal variations. This shortcoming of current knowledge in this area has prompted us to work on the development, as well as on mathematical and numerical analysis, of a novel continuum model for nanowire resonators.

In this article, we briefly describe our developed mathematical model for the vibrations of nanowire resonators. Our proposed model is based on the nonlocal Euler-Bernoulli beam theory and includes the terms related to the added mass, temperature variations, electromagnetic fields, large oscillations, and piezoelectric effect. Then, a finite difference scheme is developed to obtain the natural frequency of the nanowire resonator. Finally, a parametric sensitivity analysis is presented to show the effect of different parameters on the frequency behavior of nanowire resonators with an added mass, and the importance of nonlinearity is highlighted.

## 2 Mathematical Modelling

Utilizing the nonlocal Euler Bernoulli beam theory and incorporating different effects including surface, electromagnetic field, thermal variations, large oscillations, added mass and nonlinear foundation, the following nonlinear partial differential equation is developed for the vibrations of nanowires [9]:

$$(EI)_{eff}\frac{\partial^4 w}{\partial x^4}+\left(1-\Gamma\frac{\partial^2}{\partial x^2}\right)\Psi=0, \tag{1}$$

where

$$\begin{aligned}\Psi=(\rho A)_{eff}\frac{\partial^2 w(x,t)}{\partial t^2}+m_p\delta(x-x_p)\frac{\partial^2 w(x,t)}{\partial t^2}+\\ \mu\frac{\partial w(x,t)}{\partial t}+k_1 w(x,t)-2b\tau_0\frac{\partial^2 w}{\partial x^2}+k_3 w^3(x,t)-F(x,t)-\zeta_m A H_x^2\frac{\partial^2 w}{\partial x^2}+\\ 2V_e b e_{31}\frac{\partial^2 w}{\partial x^2}-\left(\frac{(EA)_{eff}}{2L}\int_0^L\left(\frac{\partial w}{\partial x}\right)^2 dx-N_\theta\right)\frac{\partial^2 w}{\partial x^2}.\end{aligned} \tag{2}$$

The definition of other terms presented in Eqs. (1–2) can be found in Ref. [9]. In order to solve the above partial differential equation, we develop a finite difference approximation. In the next section, we briefly describe the numerical approach applied to the solution of this problem. The considered boundary are described in Eq. (3):

$$W(0,t)=0,\ \frac{\partial W}{\partial x}(0,t)=0, W(L,t)=0, \frac{\partial W}{\partial x}(L,t)=0, \tag{3}$$

and the following general form of initial conditions are assumed:

$$W(x,t=0)=W_0, \frac{\partial W}{\partial t}(x,t=0)=\bar{W}_0, \tag{4}$$

where $W_0$ and $\bar{W}_0$ are given functions. Motivated by the applications of interest here, the model (1)–(4) is simplified in the next section. Assuming periodicity in time, we propose a solution procedure where the function $W$ will be analyzed with respect to frequency rather than time, moving our consideration to the frequency domain.

## 3 Solution Procedure

In this section we concisely illustrate the FDM in the context of our problem, and then move to the implementation of this method for the nanowire resonator.

### 3.1 FDM

Finite difference methods are a generic class of numerical methods, which are used for solving differential equations by approximating them with difference equations, where finite differences approximate the derivatives. FDMs require a discretization of the computational domain. The domain is partitioned in both space ($x$) and time ($t$), and approximations of the solution are computed at points of the grid, resulted from the domain discretization. Based on the FDM, the discretized equations for the first, second, third and fourth derivatives with respect to $x$ are as follows [10–12]:

$$\frac{\partial w}{\partial x} \approx \frac{w_{i+1} - w_{i-1}}{2\Delta x}, \quad \frac{\partial^2 w}{\partial x^2} \approx \frac{w_{i+1} - 2w_i + w_{i-1}}{(\Delta x)^2}, \tag{5}$$

$$\frac{\partial^3 w}{\partial x^3} \approx \frac{w_{i+3} - 3w_{i+2} + 3w_{i+1} - w_i}{(\Delta x)^3}, \tag{6}$$

$$\frac{\partial^4 w}{\partial x^4} \approx \frac{w_{i-2} - 4w_{i-1} + 6w_i - 4w_{i+1} + w_{i+2}}{(\Delta x)^4}, \tag{7}$$

where

$$\Delta x = \frac{Length\ of\ X}{Number\ of\ Steps\ in\ X}. \tag{8}$$

The accuracy of approximations (5) and (7) at the grid point $x_i$, is of the second order, and approximation (6) is of the first order, with respect to ($\Delta x$). In the next sub-section, we apply the FDM to our developed governing equation, Eq. (1), to allow a numerical analysis of the frequency of nanowire resonators.

### 3.2 Implementation of the FDM for the Nanowire Resonator

In this part, we apply the FDM to the governing equation (Eq. (1)) of nanowire resonators. In order to use the FDM to analyze the developed model, we assume that the displacement of the nanowire resonator can be given in the following form [10]:

$$w(x,t) = w(x)e^{i\omega t}, \tag{9}$$

where $\omega$ is the frequency of the nanowire resonator. We first consider the linear part of the developed Eq. (1) [9]. Substituting Eq. (9) into the linear part of Eq. (1) results in:

$$(P)\frac{\partial^4 w(x)}{\partial x^4} + (Q)\frac{\partial^2 w(x)}{\partial x^2} + k_1 w(x) = \bar{M}\omega^2 w(x). \tag{10}$$

By substituting the approximate derivatives, Eq. (5) and Eq. (7), into Eq. (10), the following form is obtained:

$$G_1(w_{i-2}-4w_{i-1}+6w_i-4w_{i+1}+w_{i+2})+G_2(w_{i+1}-2w_i+w_{i-1})+k_1w_i = \omega^2\big[-G_3w_i-G_4(w_{i+1}-2w_i+w_{i-1})\big], \quad (11)$$

where

$$G_1=\frac{\Big[(EI)_{eff}+2\Gamma b\tau_0+\Gamma\zeta AH_x^2+2\Gamma vbe_31+\Gamma\frac{(EA)_{eff}}{2L}N_\theta\Big]}{(\Delta x)^4}, \quad (12)$$

$$G_2=\frac{\Big[-2b\tau_0-\zeta_m AH_x^2-2vbe_31-\frac{(EA)_{eff}}{2L}N_\theta-\Gamma k_1\Big]}{(\Delta x)^2}, \quad (13)$$

$$G_3=\rho A+m_p,\quad G_4=\Gamma\frac{m_p+\rho A}{\Delta x^2}, \quad (14)$$

and

$$\bar{M}=\big[-G_3w_i-G_4(w_{i+1}-2w_i+w_{i-1})\big]. \quad (15)$$

Using Eq. (8) for $i=1,\ldots,N$, we can represent $\Delta x$ as below:

$$\Delta x=\frac{L}{(N-1)}, \quad (16)$$

where $L$ is the length of the nanowire resonator. By considering clamped-clamped boundary conditions for the nanoresonator, we will have the following equations for both ends of the nanowire:

$$\text{at }\ x=0:\ w_1=0,\quad \&\quad \frac{w_2-w_0}{2\Delta x}=0, \quad (17)$$

and

$$\text{at }\ x=N:\ w_N=0,\quad \&\quad \frac{w_{N+1}-w_{N-1}}{2\Delta x}=0. \quad (18)$$

Based on Eqs. (17) and (18), we obtain the following relations:

$$w_0=w_2,\qquad\qquad w_{N+1}=w_{N-1}. \quad (19)$$

It should be mentioned that $w_0$ and $w_{N+1}$ are fictitious values which can be eliminated in our governing equation by using Eq. (19). Now, in order to solve Eq. (10) using the FDM, we substitute $i=2,\ldots,N-1$ into Eq. (11), which results in a system of equations as follows:

$$\begin{bmatrix} A_1 & B_1 & C_1 & 0 & \dots & 0 & 0 & 0 & 0 \\ A_2 & B_2 & C_2 & D_2 & \dots & 0 & 0 & 0 & 0 \\ . & . & . & . & \dots & . & . & . & . \\ . & . & . & . & \dots & . & . & . & . \\ . & . & . & . & \dots & . & . & . & . \\ 0 & 0 & 0 & 0 & \dots & A_{N-3} & B_{N-3} & C_{N-3} & D_{N-3} \\ 0 & 0 & 0 & 0 & \dots & 0 & A_{N-2} & B_{N-2} & C_{N-2} \end{bmatrix} \begin{bmatrix} w_2 \\ w_3 \\ . \\ . \\ . \\ w_{N-2} \\ w_{N-1} \end{bmatrix} = \omega^2 \tag{20}$$

$$\begin{bmatrix} G_3 - 2G_4 & G_4 & \dots & 0 & 0 \\ G_4 & G_3 - 2G_4 & \dots & 0 & 0 \\ . & . & \dots & . & . \\ . & . & \dots & . & . \\ . & . & \dots & . & . \\ 0 & 0 & \dots & G_3 - 2G_4 & G_4 \\ 0 & 0 & \dots & G_4 & G_3 - 2G_4 \end{bmatrix} \begin{bmatrix} w_2 \\ w_3 \\ . \\ . \\ . \\ w_{N-2} \\ w_{N-1} \end{bmatrix},$$

where

$$A_1 = 7G_1 - 2G_2 + k_1, \quad B_1 = -4G_1 + G_2, \quad C_1 = G_1, \tag{21}$$

$$A_2 = -4G_1 + G_2, \quad B_2 = 4G_1 - 2G_2 + k_1, \quad C_2 = -4G_1 + G_2, \quad D_2 = G_1, \tag{22}$$

$$\begin{gathered} A_{N-3} = G_1, \quad B_{N-3} = -4G_1 + G_2, \\ C_{N-3} = 6G_1 - 2G_2 + k_1, \quad D_{N-3} = -4G_1 + G_2, \end{gathered} \tag{23}$$

and

$$A_{N-2} = G_1, \quad B_{N-2} = -4G_1 + G_2, \quad C_{N-2} = 7G_1 - 2G_2 + k_1. \tag{24}$$

Hence, Eq. (20) can be rewritten in the following form:

$$\big( -[\bar{M}]\omega^2 + [K] \big)\{w\} = 0, \tag{25}$$

where $w = \{w_2, w_3, \dots w_{N-2}, w_{N-1}\}^T$, $\bar{M}$ and K are the mass and stiffness matrices, respectively. $\bar{M}$ is defined by the following matrix:

$$\bar{M} = \begin{bmatrix} G_3 - 2G_4 & G_4 & \dots & 0 & 0 \\ G_4 & G_3 - 2G_4 & \dots & 0 & 0 \\ . & . & \dots & . & . \\ . & . & \dots & . & . \\ . & . & \dots & . & . \\ 0 & 0 & \dots & G_3 - 2G_4 & G_4 \\ 0 & 0 & \dots & G_4 & G_3 - 2G_4 \end{bmatrix}. \tag{26}$$

$K$ represents the stiffness matrix, and it can be found as follows:

$$K = \begin{bmatrix} A_1 & B_1 & C_1 & 0 & \ldots & 0 & 0 & 0 & 0 \\ A_2 & B_2 & C_2 & D_2 & \ldots & 0 & 0 & 0 & 0 \\ . & . & . & . & \ldots & . & . & . & . \\ . & . & . & . & \ldots & . & . & . & . \\ . & . & . & . & \ldots & . & . & . & . \\ 0 & 0 & 0 & 0 & \ldots & A_{N-3} & B_{N-3} & C_{N-3} & D_{N-3} \\ 0 & 0 & 0 & 0 & \ldots & 0 & A_{N-2} & B_{N-2} & C_{N-2} \end{bmatrix}. \tag{27}$$

In order to obtain the linear frequency of the vibrations of the nanowire resonator, we need to find the solution of Eq. (25). A non-trivial solution of Eq. (25) can be obtained when the determinant of coefficient matrix equals to zero:

$$\Big|\big[-[\bar{M}]\omega^2 + [K]\big]\Big| = 0. \tag{28}$$

Based on the algorithm described above, stiffness and mass matrices can be calculated numerically. These calculated matrices are used in Eq. (28) to obtain the linear natural frequency in Eq. (25). It should be noted that the size of mass and stiffness matrices depends on the number of nodes N. For the nonlinear part of the governing equation, Eq. (1), we have:

$$NL := -\frac{EA_{eff}}{2L}\left[\int_0^L \left(\frac{\partial w(x,t)}{\partial x}\right)^2 dx\right]\frac{\partial^2 w(x,t)}{\partial x^2} + k_3 w^3(x,t) \tag{29}$$

$$-\Gamma k_3 \frac{\partial^2}{\partial x^2}[w^3(x,t)] + \Gamma \frac{EA_{eff}}{2L}\left[\int_0^L \left(\frac{\partial w(x,t)}{\partial x}\right)^2 dx\right]\frac{\partial^2 w(x,t)}{\partial x^2}.$$

The integral term in our governing equation can be approximated by the following relationship:

$$\int_0^L \left(\frac{\partial w(x,t)}{\partial x}\right)^2 dx \approx \frac{L}{2}\left[\left(\frac{\partial w(x,t)}{\partial x}\right)^2\bigg|_{i=1} + \left(\frac{\partial w(x,t)}{\partial x}\right)^2\bigg|_{i=N}\right]. \tag{30}$$

Based on the defined boundary conditions in Eqs. (17–18) and the nonlinear terms presented by Eq. (29), we have the following relation to obtain the nonlinear frequency of the considered nanowire resonator:

$$\big(-[\bar{M}]\omega^2 + [K] + [K_{NL}]\big)\{w\} = 0. \tag{31}$$

To find the nonlinear natural frequency, we first need to solve the linear equation to obtain the eigenvalues and eigenvectors. It should be noted that eigenvectors and eigenvalues represent mode shapes and the linear frequencies of vibrations, respectively. Basically, these two values are used in an iterative process to obtain the nonlinear natural frequencies. Then, we utilize the obtained solution as an initial approximation to the nonlinear equation defined by Eq. (31). By substituting the derived eigenvalues and eigenvectors into Eq. (31), and also coupling the linear and nonlinear stiffness matrices with the mass matrix, the nonlinear frequency and mode shape can be calculated [13]. Then, implementing the iteration method, the nonlinear frequency is recalculated in order to find an approximate frequency, when the iterations converge with pre-defined accuracy. In the next section, we discuss the results obtained based on the developed numerical approach.

## 4 Results and Discussion

In this section, a parametric sensitivity analysis is carried out by using the numerical solution obtained with the methodology described in the previous section, for the vibration of the nanowire resonator. All figures in this section are obtained based on Eq. (28) using parameters defined in Ref. [9] with clamped-clamped boundary conditions given by Eqs. (17) and (18). We have investigated the sensitivity of dimensionless frequency, $\bar{f_n}$, obtained by numerical simulation presented in Sect. 3 with respect to variations in temperature, piezoelectric voltage, nonlocal parameter, and the added mass. The dimensionless frequency, $\bar{f_n}$, is defined by using the following equation:

$$\bar{f_n} = \frac{\omega}{\omega_0}, \tag{32}$$

where both $\omega$ and $\omega_0$ can be obtained by using Eq. (28). The constant $\omega_0$ is the frequency of the nanoresonator without considering the effect of added mass. Figure 1a shows the effect of temperature on the frequency behavior of silicon nanowire (SiNW) resonator using Eq. (32). As this figure shows, increasing the temperature reduces the frequency value of the nanowire resonator. A linear relation is observed between the temperature rise and the frequency reduction of the nanowire reosnator. Considering the developed continuum model in our analysis, the main reason of frequency reduction is attributed to a decrease in stiffness of the nanowire as its temperature increases. Using Eq. (32) based on the FDM solution, we have performed a sensitivity analysis with respect to the piezoelectric voltage, presented in Fig. 1b. Based on this figure, increasing the piezoelectric voltage reduces the frequency of silicon nanowire resonator. Accordingly, the piezoelectric voltage can be used for adjusting the vibration behavior of the nanowire resonator. Figure 2a depicts the effect of dimensionless nonlocal parameter ($(e_0 a)/L$) on the frequency behavior of the silicon nanowire resonator. This figure has been plotted by using Eq. (32) based on the FDM solution. As the figure reveals, increasing the nonlocal parameter reduces the frequency of nanowire resonator. From this figure it can be concluded that the effect of nonlocal parameter is critical and it should be taken into account in the frequency analysis of nanoscale resonators such as nanowires.

Figure 2b shows the effect of added mass on the frequency behavior of SiNW. As this figure shows, increasing the mass of added particle reduces the frequency of SiNW resonator. This figure also demonstrates a significant potential of the nanowire

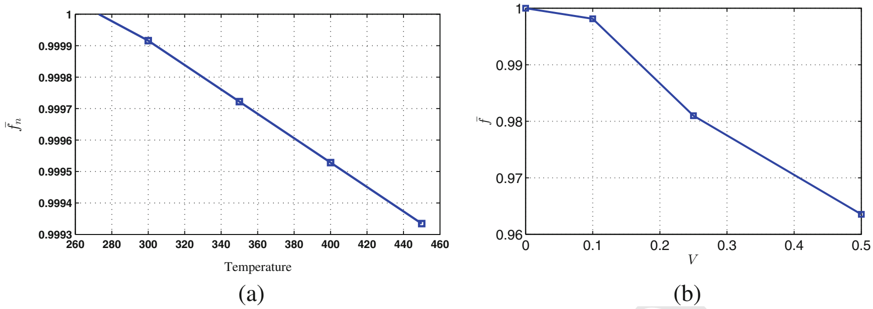


**Fig. 1** **a** Effect of temperature on the frequency behavior of SiNW using the FDM **b** effect of piezoelectric voltage on the frequency behavior of SiNW using the FDM

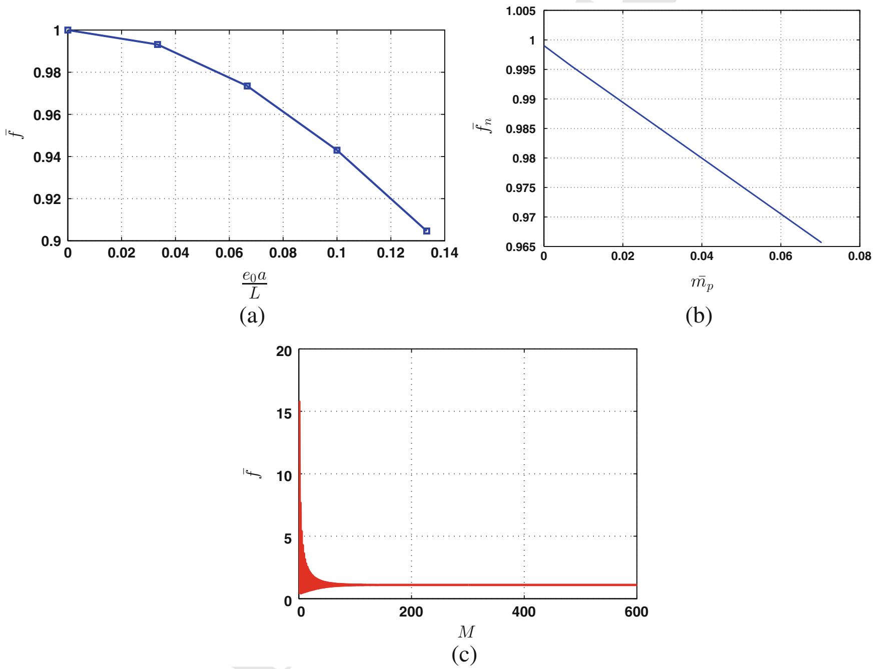


**Fig. 2** **a** Effect of dimensionless nonlocal parameter on the frequency behavior of SiNW using the FDM **b** effect of added mass on the frequency behavior of SiNW using the FDM **c** convergence analysis of the frequency response of the FDM

resonator for tiny object detection. In order to investigate the convergence of our numerical solution for the developed model of the silicon nanowire resonator, using the iterative technique in conjunction with the FDM discussed in the context of Eq. (31), we have plotted the obtained nonlinear frequency of each iteration with respect to its corresponding number of iteration, $M$. Figure 2c shows that by using the iterative technique for the nonlinear part, we can reach the convergent frequency after just a few iterations with the accuracy of $10^{-4}$.

## 5 Conclusion

In this paper, we presented a numerical solution using the FDM for the vibrations of nanowire resonator with added mass. The mathematical model for the nanowire resonator was developed based on the nonlocal Euler-Bernoulli beam theory, which includes different terms related to thermal variations, electromagnetic fields, surface and nonlocal effects, as well as added mass. It was revealed that the FDM can effectively be used to model nanoresonators and analyze their frequency of oscillations with applications to tiny mass sensing which is critical in biomedicine. It was demonstrated that an increase in temperature, piezoelectric voltage and nonlocal parameter reduces the frequency of oscillations in the nanowire resonator. In addition, adding a tiny particle, in the scale of zeptogram, in the middle of nanowire resonators results in a detectable shift in their frequency.

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