Dynamic stiffness and eigenvalues of nonlocal nano-beams

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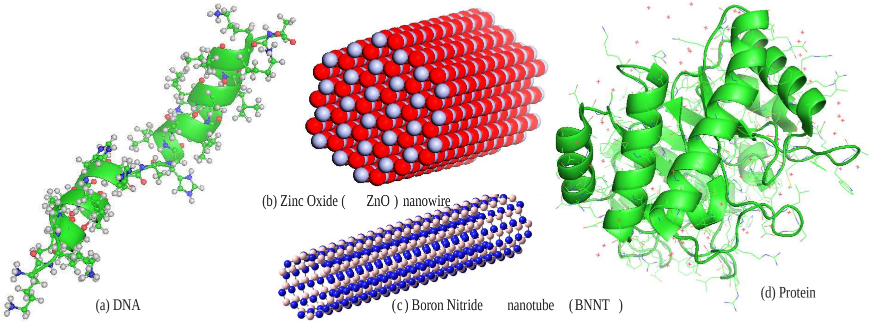
Outline of this talk

Nanoscale structures



- Nanoscale systems have length-scale in the order of $\mathcal{O}(10^{-9})$m.
- Nanoscale systems, such as those fabricated from simple and complex nanorods, nanobeams[1] and nanoplates have attracted keen interest among scientists and engineers.

Nanoscale structures

- Examples of one-dimensional nanoscale objects include (nanorod and nanobeam) carbon nanotubes[2], zinc oxide (ZnO) nanowires and boron nitride (BN) nanotubes, while two-dimensional nanoscale objects include graphene sheets[3] and BN nanosheets[4].
- These nanostructures are found to have exciting mechanical, chemical, electrical, optical and electronic properties.
- Nanostructures are being used in the field of nanoelectronics, nanodevices, nanosensors, nano-oscillators, nano-actuators, nanobearings, and micromechanical resonators, transporter of drugs, hydrogen storage, electrical batteries, solar cells, nanocomposites and nanooptomechanical systems (NOMS).
- Understanding the dynamics of nanostructures is crucial for the development of future generation applications in these areas.

Continuum mechanics at the nanoscale

- Experiments at the nanoscale are generally difficult at this point of time.
- On the other hand, atomistic computation methods such as molecular dynamic (MD) simulations[5] are computationally prohibitive for nanostructures with large numbers of atoms.
- Continuum mechanics can be an important tool for modelling, understanding and predicting physical behaviour of nanostructures.
- Although continuum models based on classical elasticity are able to predict the general behaviour of nanostructures, they often lack the accountability of effects arising from the small-scale.
- To address this, size-dependent continuum based methods[6–9] are gaining in popularity in the modelling of small sized structures as they offer much faster solutions than molecular dynamic simulations for various nano engineering problems.
- Currently research efforts are undergoing to bring in the size-effects within the formulation by modifying the traditional classical mechanics.

Nonlocal continuum mechanics

- One popularly used size-dependant theory is the nonlocal elasticity theory pioneered by Eringen[10], and has been applied to nanotechnology.
- Nonlocal continuum mechanics is being increasingly used for efficient analysis of nanostructures viz. nanorods[11,12], nanobeams[13], nanoplates[14,15], nanorings[16], carbon nanotubes[17,18], graphenes[19,20], nanoswitches[21] and microtubules[22]. Nonlocal elasticity accounts for the small-scale effects at the atomistic level.
- In the nonlocal elasticity theory the small-scale effects are captured by assuming that the stress at a point as a function of the strains at all points in the domain:

$$\sigma_{ij}(x) = \int_V \phi(|x - x'|, \alpha) t_{ij} dV(x')$$

  where $\phi(|x - x'|, \alpha) = (2\pi\ell^2\alpha^2) K_0(\sqrt{x \bullet x}/\ell\alpha)$
- Nonlocal theory considers long-range inter-atomic interactions and yields results dependent on the size of a body.
- Some of the drawbacks of the classical continuum theory could be efficiently avoided and size-dependent phenomena can be explained by the nonlocal elasticity theory.

Bending vibration of carbon nanotubes

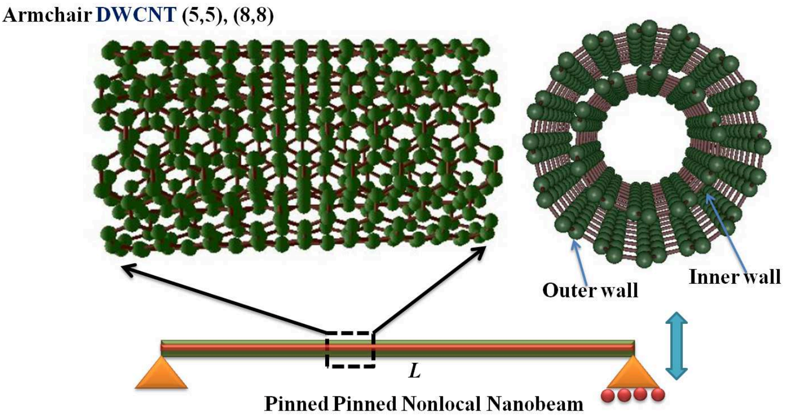


Figure: Bending vibration of an armchair (5, 5), (8, 8) double-walled carbon nanotube (DWCNT) with pinned-pinned boundary condition.

- For the bending vibration of a nonlocal damped beam, the equation of motion can be expressed by

$$EI\frac{\partial^4 V(x,t)}{\partial x^4} + m\left(1-(e_0a)^2\frac{\partial^2}{\partial x^2}\right)\left\{\frac{\partial^2 V(x,t)}{\partial t^2}\right\} = \left(1-(e_0a)^2\frac{\partial^2}{\partial x^2}\right)\{F(x,t)\} \quad (1)$$

- In the above equation EI is the bending rigidity, m is mass per unit length, e_0a is the nonlocal parameter, $V(x,t)$ is the transverse displacement and $F(x,t)$ is the applied force.
- Considering the free vibration, i.e., setting the force to zero, and assuming harmonic motion with frequency ω

$$V(x,t) = v(x)\exp[\mathrm{i}\omega t] \quad (2)$$

from (1) we have

$$EI\frac{d^4v}{dx^4} - m\omega^2\left(v-(e_0a)^2\frac{d^2v}{dx^2}\right) = 0 \quad (3)$$

$$\text{or} \quad \frac{d^4v}{dx^4} + b^4(e_0a)^2\frac{d^2v}{dx^2} - b^4v = 0 \quad (4)$$

- Here

$$b^4 = \frac{m\omega^2}{EI} \tag{5}$$

- To obtain the characteristic equation, we assume

$$v(x) = \exp[\lambda x] \tag{6}$$

- Substituting this in Eq. (4) we obtain

$$\lambda^4 + b^4(e_0 a)^2 \lambda^2 - b^4 = 0 \tag{7}$$

$$\text{or} \quad \lambda^2 = b^2 \left(-b^2(e_0 a)^2 \pm \sqrt{4 + b^4(e_0 a)^4} \right) / 2 \tag{8}$$

- Defining

$$\gamma = b^2 (e_0 a)^2 \tag{9}$$

the two roots can be expressed as

$$\lambda^2 = -\alpha^2,\ \beta^2 \tag{10}$$

- Here

$$\alpha = b\sqrt{\left(\sqrt{4+\gamma^2}+\gamma\right)/2} \tag{11}$$

$$\text{and} \quad \beta = b\sqrt{\left(\sqrt{4+\gamma^2}-\gamma\right)/2} \tag{12}$$

- Therefore, the four roots of the characteristic equation can be expressed as

$$\lambda = \mathrm{i}\alpha, -\mathrm{i}\alpha,\ \beta, -\beta \tag{13}$$

where $\mathrm{i} = \sqrt{-1}$.

- The displacement function within the beam can be expressed by linear superposition as

$$v(x) = \sum_{j=1}^{4} c_j \exp[\lambda_j x] \tag{14}$$

Here the unknown constants c_j need to be obtained from the boundary conditions.
Using Eq. (14), the natural frequency of the system can be obtained by imposing the necessary boundary conditions[23]. For example, the bending moment and shear force are given by:

  - Bending moment at $x = 0$ or $x = L$:

$$EI\frac{d^2 v(x)}{dx^2} = 0 \tag{15}$$

  - Shear force at $x = 0$ or $x = L$:

$$EI\frac{d^3 v(x)}{dx^3} + m\omega^2 (e_0 a)^2 \frac{dv(x)}{dx} = 0 \quad \text{or} \quad \frac{d^3 v(x)}{dx^3} + b^4 (e_0 a)^2 \frac{dv(x)}{dx} = 0 \tag{16}$$

Pinned-pinned nonlocal beams

- Undamped nonlocal natural frequencies of pinned-pinned nonlocal beams can be obtained[11] as

$$\lambda_j = \frac{\beta_j^2}{\sqrt{1+\beta_j^2(e_0 a)^2}}\sqrt{\frac{EI}{m}} \quad \text{where} \quad \beta_j = j\pi/L, \quad j = 1, 2, \cdots \tag{17}$$

- Asymptotic behaviour: For higher order modes $j \to \infty$ we can show that

$$\lambda_j \to \frac{\beta_j}{(e_0 a)}\sqrt{\frac{EI}{m}} \quad j = 1, 2, \cdots \tag{18}$$

  Unlike conventional 'local beams' where frequencies increase as square of the mode count j, for nonlocal beams the frequencies increase linearly with j[1].

[1] Lei, Y., Murmu, T., Adhikari, S. and Friswell, M. I., "Asymptotic frequencies of damped nonlocal beams and plates", Mechanics Research Communication, to appear.

Conventional finite element method for nonlocal beams

- We consider an element of length ℓ_e with bending stiffness EI and mass per unit length m.

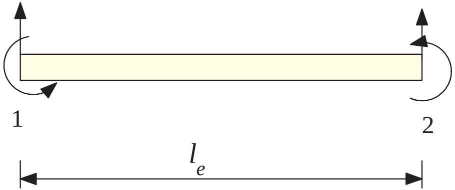


Figure: A nonlocal element for the bending vibration of a beam. It has two nodes and four degrees of freedom. The displacement field within the element is expressed by cubic shape functions.

- This element has four degrees of freedom and there are four shape functions.

- The shape function matrix for the bending deformation[24] can be given by

$$\mathbf{N}(x) = [N_1(x), N_2(x), N_3(x), N_4(x)]^T \tag{19}$$

where

$$\begin{aligned} N_1(x) &= 1 - 3\frac{x^2}{\ell_e^2} + 2\frac{x^3}{\ell_e^3}, & N_2(x) &= x - 2\frac{x^2}{\ell_e} + \frac{x^3}{\ell_e^2}, \\ N_3(x) &= 3\frac{x^2}{\ell_e^2} - 2\frac{x^3}{\ell_e^3}, & N_4(x) &= -\frac{x^2}{\ell_e} + \frac{x^3}{\ell_e^2} \end{aligned} \tag{20}$$

- Using this, the stiffness matrix can be obtained using the conventional variational formulation[25] as

$$\mathbf{K}_e = EI \int_0^{\ell_e} \frac{d^2\mathbf{N}(x)}{dx^2} \frac{d^2\mathbf{N}^T(x)}{dx^2} \mathrm{d}x = \frac{EI}{\ell_e^3} \begin{bmatrix} 12 & 6\ell_e & -12 & 6\ell_e \\ 6\ell_e & 4\ell_e^2 & -6\ell_e & 2\ell_e^2 \\ -12 & -6\ell_e & 12 & -6\ell_e^2 \\ 6\ell_e & 2\ell_e^2 & -6\ell_e & 4\ell_e^2 \end{bmatrix} \tag{21}$$

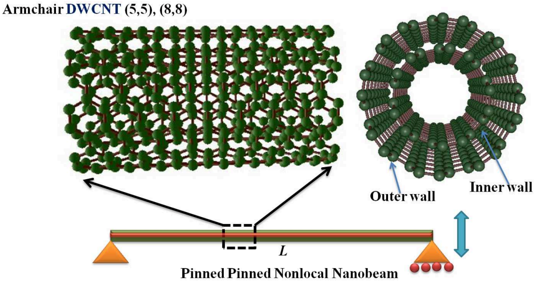
Nonlocal element mass matrix

- The mass matrix for the nonlocal element can be obtained as

$$\mathbf{M}_e = m\int_0^{\ell_e} \mathbf{N}(x)\mathbf{N}^T(x)\mathrm{d}x + m(e_0a)^2 \int_0^{\ell_e} \frac{d\mathbf{N}(x)}{dx}\frac{d\mathbf{N}^T(x)}{dx}\mathrm{d}x$$
$$= \frac{m\ell_e}{420}\begin{bmatrix} 156 & 22\ell_e & 54 & -13\ell_e \\ 22\ell_e & 4\ell_e^2 & 13\ell_e & -3\ell_e^2 \\ 54 & 13\ell_e & 156 & -22\ell_e \\ -13\ell_e & -3\ell_e^2 & -22\ell_e & 4\ell_e^2 \end{bmatrix}$$
$$+\left(\frac{e_0a}{\ell_e}\right)^2 \frac{m\ell_e}{30}\begin{bmatrix} 36 & 3\ell_e & -36 & 3\ell_e \\ 3\ell_e & 4\ell_e^2 & -3\ell_e & -\ell_e^2 \\ -36 & -3\ell_e & 36 & -3\ell_e \\ 3\ell_e & -\ell_e^2 & -3\ell_e & 4\ell_e^2 \end{bmatrix} \quad (22)$$

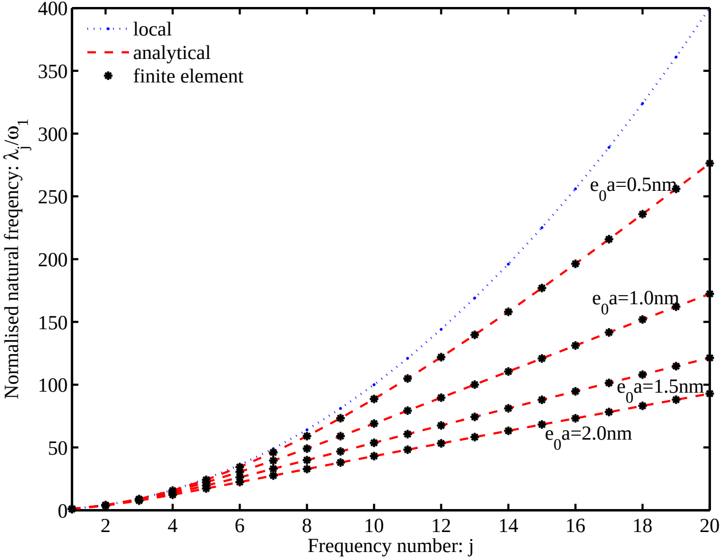
- For the special case when the beam is local, the mass matrix derived above reduces to the classical mass matrix[24,25] as $e_0a = 0$.

Bending vibration of a double-walled carbon nanotube



- A double-walled carbon nanotube (DWCNT) is considered.
- An armchair (5, 5), (8, 8) DWCNT with Young's modulus $E = 1.0$ TPa, $L = 30$ nm, density $\rho = 2.3 \times 10^3$ kg/m^3 and thickness t = 0.35 nm is used
- The inner and the outer diameters of the DWCNT are respectively 0.68nm and 1.1nm.
- We consider pinned-pinned boundary condition.
- For the finite element analysis the DWCNT is divided into 100 elements. The dimension of each of the system matrices become 200×200, that is $n = 200$.

Nonlocal natural frequencies of DWCNT



First 20 undamped natural frequencies for the axial vibration of SWCNT.

- For the bending vibration of a nonlocal damped beam, the equation of motion can be expressed by

$$EI\frac{\partial^4 V(x,t)}{\partial x^4} + m\left(1-(e_0a)^2\frac{\partial^2}{\partial x^2}\right)\left\{\frac{\partial^2 V(x,t)}{\partial t^2}\right\} + \widehat{c}_1\frac{\partial^5 V(x,t)}{\partial x^4 \partial t} + \widehat{c}_2\frac{\partial V(x,t)}{\partial t} = \left(1-(e_0a)^2\frac{\partial^2}{\partial x^2}\right)\{F(x,t)\} \quad (23)$$

- In the above equation EI is the bending rigidity, m is mass per unit length, e_0a is the nonlocal parameter, $V(x,t)$ is the transverse displacement and $F(x,t)$ is the applied force.
- The constant $\widehat{c}_1$ is the strain-rate-dependent viscous damping coefficient and $\widehat{c}_2$ is the velocity-dependent viscous damping coefficient.
- Following the damping convention in dynamic analysis[23], we consider stiffness and mass proportional damping. Therefore, we express the damping constants as

$$\widehat{c}_1 = \zeta_1(EI) \quad \text{and} \quad \widehat{c}_2 = \zeta_2(m) \quad (24)$$

where ζ_1 and ζ_2 are stiffness and mass proportional damping factors.

- Considering the free vibration, i.e., setting the force to zero, and assuming harmonic motion with frequency ω

$$V(x,t) = v(x)\exp\left[\mathrm{i}\omega t\right] \tag{25}$$

from Eq. (23) we have

$$EI\frac{d^4 v}{dx^4} - m\omega^2\left(v - (e_0 a)^2\frac{d^2 v}{dx^2}\right) + \mathrm{i}\omega\widehat{c}_1\frac{d^4 v}{dx^4} + \mathrm{i}\omega\widehat{c}_2 v = 0 \tag{26}$$

- Using the damping factors, from Eq. (26) we have

$$EI\left(1+\mathrm{i}\omega\zeta_1\right)\frac{d^4 v}{dx^4} + m\omega^2(e_0 a)^2\frac{d^2 v}{dx^2} - m\omega^2\left(1-\mathrm{i}\zeta_2/\omega\right)v = 0 \tag{27}$$

$$\text{or}\quad \frac{d^4 v}{dx^4} + \bar{b}^4(e_0 a)^2\frac{d^2 v}{dx^2} - \bar{b}^4\theta v = 0 \tag{28}$$

where we define $\bar{b}$ and introduce θ as

$$\bar{b}^4 = \frac{m\omega^2}{EI\left(1+\mathrm{i}\omega\zeta_1\right)} \quad \text{and} \quad \theta = \left(1-\mathrm{i}\zeta_2/\omega\right) \tag{29}$$

- To obtain the characteristic equation, we assume

$$v(x) = \exp\left[\lambda x\right] \tag{30}$$

- Substituting this in Eq. (28) we obtain

$$\lambda^4 + \bar{b}^4 (e_0 a)^2 \lambda^2 - \bar{b}^4 \theta = 0 \tag{31}$$

- Defining

$$\gamma = \bar{b}^2 (e_0 a)^2 \tag{32}$$

  the two roots can be expressed as

$$\lambda^2 = -\alpha^2,\ \beta^2 \tag{33}$$

- The expressions of α and β are given by

$$\alpha = \bar{b}\sqrt{\left(\sqrt{4\theta + \gamma^2} + \gamma\right)/2} \tag{34}$$

and

$$\beta = \bar{b}\sqrt{\left(\sqrt{4\theta + \gamma^2} - \gamma\right)/2} \tag{35}$$

- Therefore, the four roots of the characteristic equation can be expressed as

$$\lambda = \mathrm{i}\alpha, -\mathrm{i}\alpha,\ \beta, -\beta \tag{36}$$

where $\mathrm{i} = \sqrt{-1}$.

Nonlocal element matrix

- We consider an element of length L with bending stiffness EI and mass per unit length m.

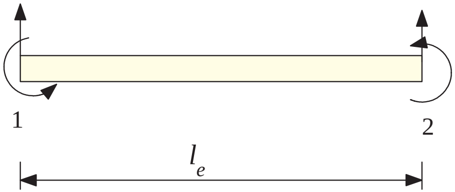


Figure: A nonlocal element for the bending vibration of a beam. It has two nodes and four degrees of freedom. The displacement field within the element is expressed by complex frequency dependent functions.

Dynamic shape functions

- The undimmed dynamic stiffness matrix can be obtained using the displacement and force boundary conditions using Banerjee's method[26]
- We propose an approach using complex shape functions which is suitable for damped systems
- Similarly to the classical finite element method, assume that the frequency-dependent displacement within an element is interpolated from the nodal displacements as

$$v_e(x,\omega) = \mathbf{N}^T(x,\omega)\widehat{\mathbf{v}}_e(\omega) \tag{37}$$

- Here $\widehat{\mathbf{v}}_e(\omega) \in \mathbb{C}^n$ is the nodal displacement vector $\mathbf{N}(x,\omega) \in \mathbb{C}^n$ is the vector of frequency-dependent shape functions and $n = 4$ is the number of the nodal degrees-of-freedom.
- Suppose the $s_j(x,\omega) \in \mathbb{C}, j = 1, \cdots, 4$ are the basis functions which exactly satisfy Eq. (28). It can be shown that the shape function vector can be expressed as

$$\mathbf{N}(x,\omega) = \mathbf{\Gamma}(\omega)\mathbf{s}(x,\omega) \tag{38}$$

where the vector $\mathbf{s}(x,\omega) = \left\{s_j(x,\omega)\right\}^T, \forall j = 1, \cdots, 4$ and the complex matrix $\mathbf{\Gamma}(\omega) \in \mathbb{C}^{4\times4}$ depends on the boundary conditions.

- The elements of $\mathbf{s}(x, \omega)$ constitutes $\exp[\lambda_j x]$ where the values of λ_j are obtained from the solution of the characteristics equation as given in Eq. (36).
- An element for the damped beam under bending vibration is shown in 3. The degrees-of-freedom for each nodal point include a vertical and a rotational degrees-of-freedom.
- In view of the solutions in Eq. (36), the displacement field with the element can be expressed by linear combination of the basic functions $e^{-\mathrm{i}\alpha x}$, $e^{\mathrm{i}\alpha x}$, $e^{\beta x}$ and $e^{-\beta x}$.
- Therefore, in our notations $\mathbf{s}(x, \omega) = \left\{e^{-\mathrm{i}\alpha x}, e^{\mathrm{i}\alpha x}, e^{\beta x}, e^{-\beta x}\right\}^T$.

- We can also express $\mathbf{s}(x,\omega)$ in terms of trigonometric functions. Considering $e^{\pm \mathrm{i}\alpha x} = \cos(\alpha x) \pm \mathrm{i}\sin(\alpha x)$ and $e^{\pm \beta x} = \cosh(\beta x) \pm \mathrm{i}\sinh(\beta x)$, the vector $\mathbf{s}(x,\omega)$ can be alternatively expressed as

$$\mathbf{s}(x,\omega) = \begin{Bmatrix} \sin(\alpha x) \\ \cos(\alpha x) \\ \sinh(\beta x) \\ \cosh(\beta x) \end{Bmatrix} \in \mathbb{C}^4 \tag{39}$$

- The displacement field within the element can be expressed as

$$v(x) = \mathbf{s}(x,\omega)^T \mathbf{v}_e \tag{40}$$

where $\mathbf{v}_e \in \mathbb{C}^4$ is the vector of constants to be determined from the boundary conditions.

Dynamic shape functions

The relationship between the shape functions and the boundary conditions can be represented as in 1, where boundary conditions in each column give rise to the corresponding shape function.

	$N_1(x,\omega)$	$N_2(x,\omega)$	$N_3(x,\omega)$	$N_4(x,\omega)$
$y(0)$	1	0	0	0
$\frac{\mathrm{d}y}{\mathrm{d}x}(0)$	0	1	0	0
$y(L)$	0	0	1	0
$\frac{\mathrm{d}y}{\mathrm{d}x}(L)$	0	0	0	1

Table: The relationship between the boundary conditions and the shape functions for the bending vibration of beams.

Closed-form expressions of the elements

- The stiffness and mass matrices can be obtained similarly to the static finite element case discussed before.
- Note that for this case all the matrices become complex and frequency-dependent. It is more convenient to define the dynamic stiffness matrix as

$$\mathbf{D}_e(\omega) = \mathbf{K}_e(\omega) - \omega^2 \mathbf{M}_e(\omega) \tag{41}$$

- The equation of dynamic equilibrium is

$$\mathbf{D}_e(\omega)\widehat{\mathbf{v}}_e(\omega) = \widehat{\mathbf{f}}(\omega) \tag{42}$$

- In Eq. (41), the frequency-dependent stiffness and mass matrices can be obtained as

$$\mathbf{K}_e(\omega) = EI \int_0^L \frac{d^2\mathbf{N}(x,\omega)}{dx^2} \frac{d^2\mathbf{N}^T(x,\omega)}{dx^2} \mathrm{d}x \tag{43}$$

$$\text{and} \quad \mathbf{M}_e(\omega) = m \int_0^L \mathbf{N}(x,\omega)\mathbf{N}^T(x,\omega) \mathrm{d}x \tag{44}$$

After some algebraic simplifications[27,28] it can be shown that the dynamic stiffness matrix is given by the following closed-form expression

$$\mathbf{D}_e(\omega) = EI\Delta \times$$
$$\begin{bmatrix} -\alpha\beta\left(cS\beta + Cs\alpha\right) & \beta\left(c\alpha C - \alpha - sS\beta\right) & \alpha\beta\left(S\beta + s\alpha\right) & -\left(C - c\right)\alpha\beta \\ \beta\left(c\alpha C - \alpha - sS\beta\right) & -sC\beta + c\alpha S & \left(C - c\right)\alpha\beta & -\alpha S + s\beta \\ \alpha\beta\left(S\beta + s\alpha\right) & \left(C - c\right)\alpha\beta & -\alpha\beta\left(cS\beta + Cs\alpha\right) & \alpha\left(s\alpha S - \beta + cC\beta\right) \\ -\left(C - c\right)\alpha\beta & -\alpha S + s\beta & \alpha\left(s\alpha S - \beta + cC\beta\right) & -sC\beta + c\alpha S \end{bmatrix}$$

where

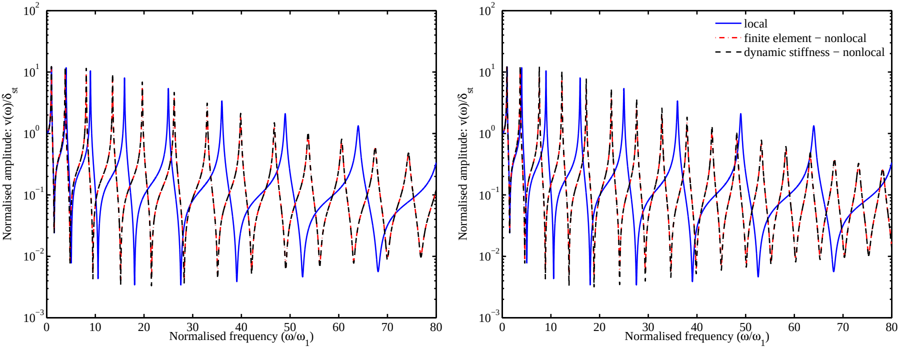
$$\Delta = \frac{(\alpha^2 + \beta^2)}{sS(\alpha^2 - \beta^2) - 2\alpha\beta(1 - cC)} \tag{45}$$

with

$$C = \cosh(\beta L), \quad c = \cos(\alpha L), \quad S = \sinh(\beta L) \quad \text{and} \quad s = \sin(\alpha L) \tag{46}$$

These are frequency dependent complex quantities because α and β are functions of ω and damping factors.

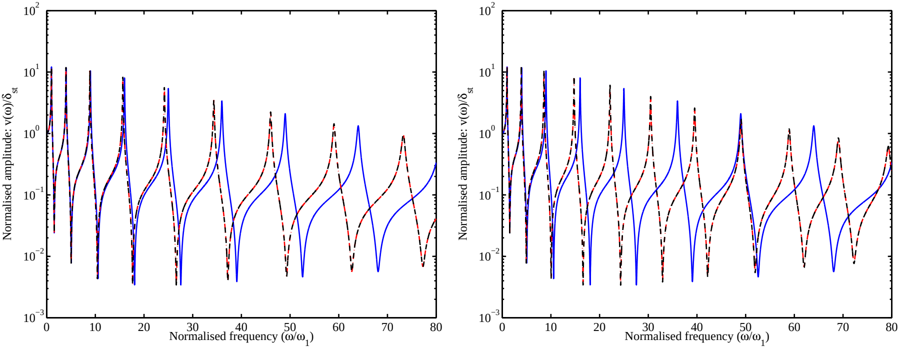
Dynamic response analysis



(a) $e_0 a = 1.5$nm (b) $e_0 a = 2.0$nm

Figure: Amplitude of the normalised frequency response of the DWCNT $v(\omega)$ at the right-end ($\zeta_2 = 0.05$ and $\zeta_1 = 10^{-4}$).

Dynamic response analysis



(a) $e_0a = 0.5$nm (b) $e_0a = 1.0$nm

Figure: Amplitude of the normalised frequency response of the DWCNT $v(\omega)$ at the right-end ($\zeta_2 = 0.05$ and $\zeta_1 = 10^{-4}$).

Conclusions

- A dynamic finite element approach for bending vibration of damped nonlocal beams is proposed.
- Strain rate dependent viscous damping and velocity dependent viscous damping are considered. Damped and undamped dynamics are discussed.
- Frequency dependent complex-valued shape functions are used to obtain the dynamic stiffness matrix in closed-form.
- The proposed method is numerically applied to the bending vibration of an armchair (5, 5), (8, 8) double-walled carbon nanotube with pinned-pinned boundary condition.
- The natural frequencies and the dynamic response obtained using the conventional finite element approach were compared with the results obtained using the dynamic stiffness method.
- Good agreement between conventional finite element with 100 elements and proposed dynamic finite element with only 1 element was found.
- This demonstrated the accuracy and computational efficiency of the proposed dynamic stiffness method in the context of nano scale structures.

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