# Dynamics of nonlocal structures

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**Outline of this talk**

## Nanoscale systems

- 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.
- 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.

(a) DNA

(b) Zinc Oxide ( ZnO ) nanowire

(c ) Boron Nitride nanotube ( BNNT )

(d) Protein
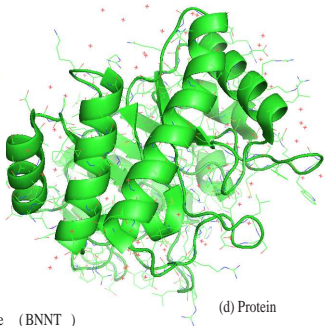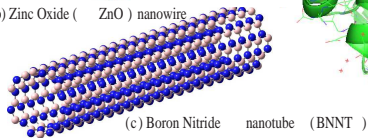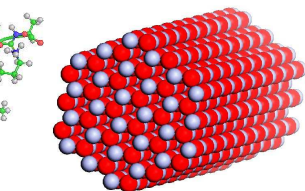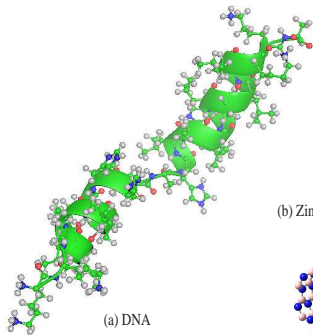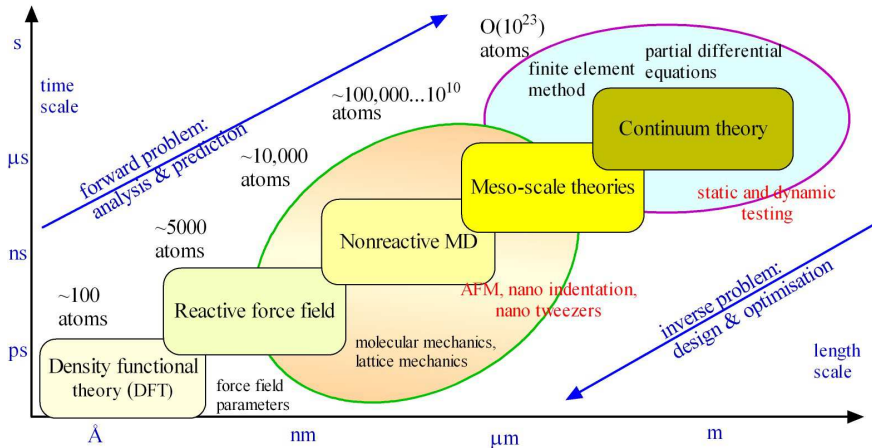
- Experiments at the nanoscale are generally difficult at this point of time.
- On the other hand, atomistic computation methods such as molecular dynamic (MD) simulations [5] are computationally prohibitive for nanostructures with large numbers of atoms.
- Continuum mechanics can be an important tool 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:

$$\sigma_{ij}(x) = \int_V \phi(|x - x'|, \alpha) t_{ij} dV(x')$$
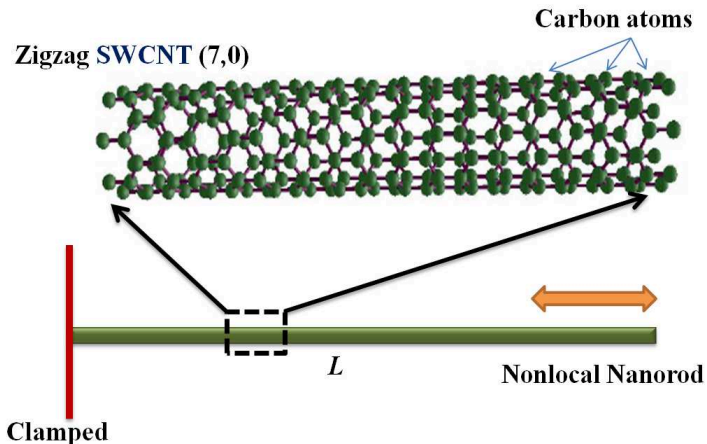
  where $\phi(|x - x'|, \alpha) = (2\pi \ell^2 \alpha^2) K_0(\sqrt{x \bullet x}/\ell \alpha)$

- 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.

- The majority of the reported works on nonlocal finite element analysis consider free vibration studies where the effect of non-locality on the undamped eigensolutions has been studied.
- Damped nonlocal systems and forced vibration response analysis have received little attention.
- On the other hand, significant body of literature is available [23–25] on finite element analysis of local dynamical systems.
- It is necessary to extend the ideas of local modal analysis to nonlocal systems to gain qualitative as well as quantitative understanding.
- This way, the dynamic behaviour of general nonlocal discretised systems can be explained in the light of well known established theories of discrete local systems.

**Figure :** Axial vibration of a zigzag (7, 0) single-walled carbon nanotube (SWCNT) with clamped-free boundary condition.

## Axial vibration of nanorods

- The equation of motion of axial vibration for a damped nonlocal rod can be expressed as

$$
EA\frac{\partial^2 U(x,t)}{\partial x^2} + \widehat{c}_1 \left(1 - (e_0 a)_1^2 \frac{\partial^2}{\partial x^2}\right) \frac{\partial^3 U(x,t)}{\partial x^2 \partial t}
$$
$$
= \widehat{c}_2 \left(1 - (e_0 a)_2^2 \frac{\partial^2}{\partial x^2}\right) \frac{\partial U(x,t)}{\partial t} + \left(1 - (e_0 a)^2 \frac{\partial^2}{\partial x^2}\right) \left\{ m\frac{\partial^2 U(x,t)}{\partial t^2} + F(x,t) \right\}
$$

- In the above equation $EA$ is the axial rigidity, $m$ is mass per unit length, $e_0 a$ is the nonlocal parameter [10], $U(x,t)$ is the axial displacement, $F(x,t)$ is the applied force, $x$ is the spatial variable and $t$ is the time.
- The constant $\widehat{c}_1$ is the strain-rate-dependent viscous damping coefficient and $\widehat{c}_2$ is the velocity-dependent viscous damping coefficient.
- The parameters $(e_0 a)_1$ and $(e_0 a)_2$ are nonlocal parameters related to the two damping terms, which are ignored for simplicity.

- We consider an element of length $\ell_e$ with axial stiffness *EA* and mass per unit length *m*.
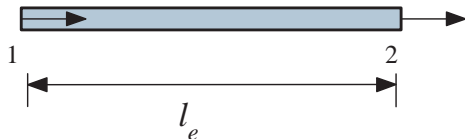


**Figure :** A nonlocal element for the axially vibrating rod with two nodes. It has two degrees of freedom and the displacement field within the element is expressed by linear shape functions.

- This element has two degrees of freedom and there are two shape functions $N_1(x)$ and $N_2(x)$. The shape function matrix for the axial deformation [25] can be given by

$$\mathbf{N}(x) = [N_1(x), N_2(x)]^T = [1 - x/\ell_e, x/\ell_e]^T \qquad (2)$$

- Using this the stiffness matrix can be obtained using the conventional variational formulation as

$$\mathbf{K}_e = EA \int_0^{\ell_e} \frac{d\mathbf{N}(x)}{dx} \frac{d\mathbf{N}^T(x)}{dx} \mathrm{d}x = \frac{EA}{\ell_e} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{3}$$

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

$$
\begin{aligned}
\mathbf{M}_e &= m \int_0^{\ell_e} \mathbf{N}(x)\mathbf{N}^T(x)\mathrm{d}x + m(e_0 a)^2 \int_0^{\ell_e} \frac{d\mathbf{N}(x)}{dx} \frac{d\mathbf{N}^T(x)}{dx} \mathrm{d}x \\
&= \frac{m\ell_e}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} + \left( \frac{e_0 a}{\ell_e} \right)^2 m\ell_e \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}
\end{aligned}
\tag{4}
$$

- For the special case when the rod is local, the mass matrix derived above reduces to the classical mass matrix[25, 26] as $e_0 a = 0$ . Therefore for a nonlocal rod, the element stiffness matrix is identical to that of a classical local rod but the element mass has an additive term which is dependent on the nonlocal parameter.
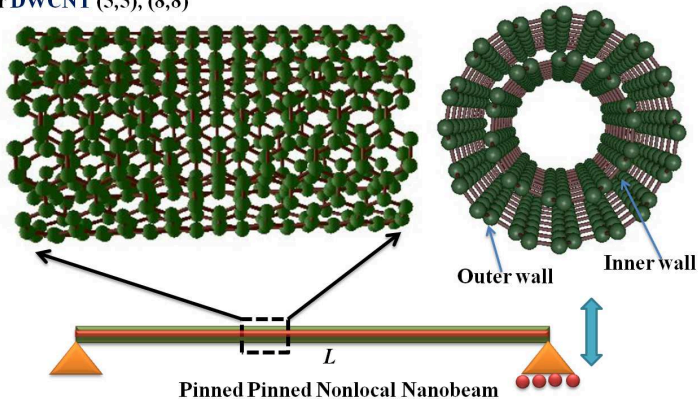
**Figure :** Bending vibration of an armchair (5, 5), (8, 8) double-walled carbon nanotube (DWCNT) with pinned-pinned boundary condition.

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

$$
EI\frac{\partial^4 V(x,t)}{\partial x^4} + m\left(1 - (e_0 a)^2 \frac{\partial^2}{\partial x^2}\right)\left\{\frac{\partial^2 V(x,t)}{\partial t^2}\right\}
$$
$$
+ \widehat{c}_1\frac{\partial^5 V(x,t)}{\partial x^4 \partial t} + \widehat{c}_2\frac{\partial V(x,t)}{\partial t} = \left(1 - (e_0 a)^2 \frac{\partial^2}{\partial x^2}\right)\{F(x,t)\} \quad (5)
$$

- In the above equation $EI$ is the bending rigidity, $m$ is mass per unit length, $e_0 a$ 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.

- We consider an element of length $\ell_e$ with bending stiffness *EI* and mass per unit length *m*.
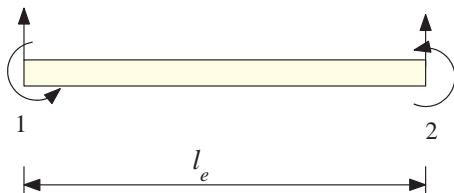


**Figure :** A nonlocal element for the bending vibration of a beam. It has two nodes and four degrees of freedom. The displacement field within the element is expressed by cubic shape functions.

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

- The shape function matrix for the bending deformation [25] can be given by

$$\mathbf{N}(x) = [N_1(x), N_2(x), N_3(x), N_4(x)]^T \tag{6}$$

where

$$
\begin{aligned}
N_1(x) &= 1 - 3\frac{x^2}{\ell_e^2} + 2\frac{x^3}{\ell_e^3}, & N_2(x) &= x - 2\frac{x^2}{\ell_e} + \frac{x^3}{\ell_e^2}, \\
N_3(x) &= 3\frac{x^2}{\ell_e^2} - 2\frac{x^3}{\ell_e^3}, & N_4(x) &= -\frac{x^2}{\ell_e} + \frac{x^3}{\ell_e^2}
\end{aligned}
\tag{7}
$$

- Using this, the stiffness matrix can be obtained using the conventional variational formulation [26] as

$$\mathbf{K}_e = EI \int_0^{\ell_e} \frac{d^2\mathbf{N}(x)}{dx^2}\frac{d^2\mathbf{N}^T(x)}{dx^2}\mathrm{d}x = \frac{EI}{\ell_e^3}\begin{bmatrix} 12 & 6\ell_e & -12 & 6\ell_e \\ 6\ell_e & 4\ell_e^2 & -6\ell_e & 2\ell_e^2 \\ -12 & -6\ell_e & 12 & -6\ell_e^2 \\ 6\ell_e & 2\ell_e^2 & -6\ell_e & 4\ell_e^2 \end{bmatrix} \tag{8}$$

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

$$
\begin{aligned}
\mathbf{M}_e &= m \int_0^{\ell_e} \mathbf{N}(x)\mathbf{N}^T(x)\mathrm{d}x + m(e_0 a)^2 \int_0^{\ell_e} \frac{d\mathbf{N}(x)}{dx}\frac{d\mathbf{N}^T(x)}{dx}\mathrm{d}x \\
&= \frac{m\ell_e}{420}
\begin{bmatrix}
156 & 22\ell_e & 54 & -13\ell_e \\
22\ell_e & 4\ell_e^2 & 13\ell_e & -3\ell_e^2 \\
54 & 13\ell_e & 156 & -22\ell_e \\
-13\ell_e & -3\ell_e^2 & -22\ell_e & 4\ell_e^2
\end{bmatrix} \\
&\quad + \left(\frac{e_0 a}{\ell_e}\right)^2 \frac{m\ell_e}{30}
\begin{bmatrix}
36 & 3\ell_e & -36 & 3\ell_e \\
3\ell_e & 4\ell_e^2 & -3\ell_e & -\ell_e^2 \\
-36 & -3\ell_e & 36 & -3\ell_e \\
3\ell_e & -\ell_e^2 & -3\ell_e & 4\ell_e^2
\end{bmatrix}
\end{aligned}
\tag{9}
$$

- For the special case when the beam is local, the mass matrix derived above reduces to the classical mass matrix [25, 26] as $e_0 a = 0$.

SL-Graphene

Carbon atoms

$W$

$L$
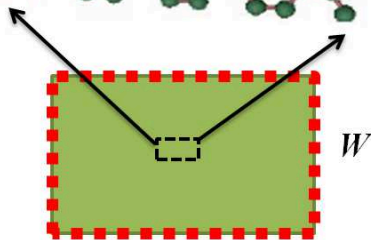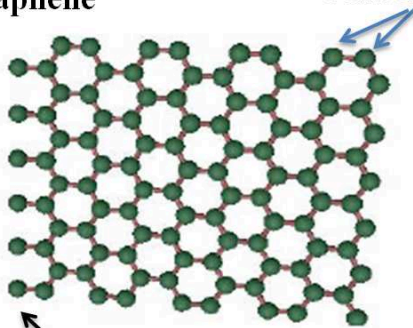
Simply-supported          Nonlocal Nanoplate

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

$$D\nabla^4 V(x,y,t) + m\left(1 - (e_0 a)^2 \nabla^2\right)\left\{\frac{\partial^2 V(x,y,t)}{\partial t^2}\right\} + \widehat{c}_1 \nabla^4 \frac{\partial V(x,y,t)}{\partial t}$$

$$+ \widehat{c}_2 \frac{\partial V(x,y,t)}{\partial t} = \left(1 - (e_0 a)^2 \nabla^2\right)\left\{F(x,y,t)\right\} \quad (10)$$

- In the above equation $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$ is the differential operator, $D = \frac{Eh^3}{12(1-\nu^2)}$ is the bending rigidity, $h$ is the thickness, $\nu$ is the Poisson's ratio, $m$ is mass per unit area, $e_0 a$ is the nonlocal parameter, $V(x,y,t)$ is the transverse displacement and $F(x,y,t)$ 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.

- We consider an element of dimension $2c \times 2b$ with bending stiffness $D$ and mass per unit area $m$.
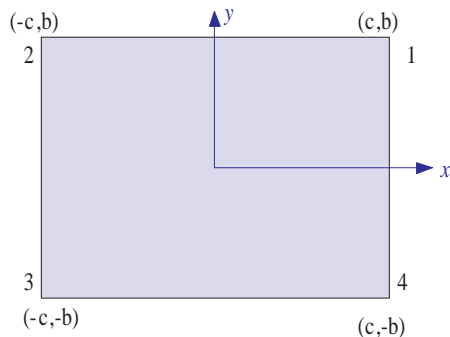


**Figure :** A nonlocal element for the bending vibration of a plate. It has four nodes and twelve degrees of freedom. The displacement field within the element is expressed by cubic shape functions in both directions.

- The shape function matrix for the bending deformation is a $12 \times 1$ vector [26] and can be expressed as

$$\mathbf{N}(x, y) = \mathbf{C}_e^{-1} \alpha(x, y) \tag{11}$$

- Here the vector of polynomials is given by

$$\alpha(x, y) = \begin{bmatrix} 1 & x & y & x^2 & xy & y^2 & x^3 & x^2y & xy^2 & y^3 & x^3y & xy^3 \end{bmatrix}^T \tag{12}$$

- The $12 \times 12$ coefficient matrix can be obtained in closed-form.

- Using the shape functions in Eq. (11), the stiffness matrix can be obtained using the conventional variational formulation [26] as

$$\mathbf{K}_e = \int_{A_e} \mathbf{B}^T \mathbf{E} \mathbf{B} \mathrm{d} A_e \tag{13}$$

- In the preceding equation **B** is the strain-displacement matrix, and the matrix **E** is given by

$$\mathbf{E} = D \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix} \tag{14}$$

- Evaluating the integral in Eq. (13), we can obtain the element stiffness matrix in closed-form as

$$\mathbf{K}_e = \frac{Eh^3}{12(1-\nu^2)} {\mathbf{C}^{-1}}^T \mathbf{k}_e \mathbf{C}^{-1} \tag{15}$$

- The $12 \times 12$ coefficient matrix $\mathbf{k}_e$ can be obtained in closed-form.

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

$$
\begin{aligned}
\mathbf{M}_e = \rho h \int_{A_e} & \left\{ \mathbf{N}(x,y)\mathbf{N}^T(x,y) \right. \\
& \left. + (e_0 a)^2 \left( \frac{\partial \mathbf{N}(x,y)}{\partial x} \frac{d\mathbf{N}^T(x,y)}{dx} + \frac{\partial \mathbf{N}(x,y)}{\partial x} \frac{d\mathbf{N}^T(x,y)}{dx} \right) \right\} \, \mathrm{d}A_e \quad (16) \\
& = \mathbf{M}_{0_e} + \left( \frac{e_0 a}{c} \right)^2 \mathbf{M}_{x_e} + \left( \frac{e_0 a}{b} \right)^2 \mathbf{M}_{y_e}
\end{aligned}
$$

- The three matrices appearing in the above expression can be obtained in closed-form.

# Nonlocal element matrices

$$\mathbf{M}_{xe} = \frac{\rho hcb}{630} \times$$

$$
\begin{bmatrix}
276 & 66b & 42c & -276 & -66b & 42c & -102 & 39b & 21c & 102 & -39b & 21c \\
66b & 24b^2 & 0 & -66b & -24b^2 & 0 & -39b & 18b^2 & 0 & 39b & -18b^2 & 0 \\
42c & 0 & 112c^2 & -42c & 0 & -28c^2 & -21c & 0 & -14c^2 & 21c & 0 & 56c^2 \\
-276 & -66b & -42c & 276 & 66b & -42c & 102 & -39b & -21c & -102 & 39b & -21c \\
-66b & -24b^2 & 0 & 66b & 24b^2 & 0 & 39b & -18b^2 & 0 & -39b & 18b^2 & 0 \\
42c & 0 & -28c^2 & -42c & 0 & 112c^2 & -21c & 0 & 56c^2 & 21c & 0 & -14c^2 \\
-102 & -39b & -21c & 102 & 39b & -21c & 276 & -66b & -42c & -276 & 66b & -42c \\
39b & 18b^2 & 0 & -39b & -18b^2 & 0 & -66b & 24b^2 & 0 & 66b & -24b^2 & 0 \\
21c & 0 & -14c^2 & -21c & 0 & 56c^2 & -42c & 0 & 112c^2 & 42c & 0 & -28c^2 \\
102 & 39b & 21c & -102 & -39b & 21c & -276 & 66b & 42c & 276 & -66b & 42c \\
-39b & -18b^2 & 0 & 39b & 18b^2 & 0 & 66b & -24b^2 & 0 & -66b & 24b^2 & 0 \\
21c & 0 & 56c^2 & -21c & 0 & -14c^2 & -42c & 0 & -28c^2 & 42c & 0 & 112c^2
\end{bmatrix}
\tag{17}
$$

$$\mathbf{M}_{ye} = \frac{\rho hcb}{630} \times$$

$$
\begin{bmatrix}
276 & 42b & 66c & 102 & 21b & -39c & -102 & 21b & 39c & -276 & 42b & -66c \\
42b & 112b^2 & 0 & 21b & 56b^2 & 0 & -21b & -14b^2 & 0 & -42b & -28b^2 & 0 \\
66c & 0 & 24c^2 & 39c & 0 & -18c^2 & -39c & 0 & 18c^2 & -66c & 0 & -24c^2 \\
102 & 21b & 39c & 276 & 42b & -66c & -276 & 42b & 66c & -102 & 21b & -39c \\
21b & 56b^2 & 0 & 42b & 112b^2 & 0 & -42b & -28b^2 & 0 & -21b & -14b^2 & 0 \\
-39c & 0 & -18c^2 & -66c & 0 & 24c^2 & 66c & 0 & -24c^2 & 39c & 0 & 18c^2 \\
-102 & -21b & -39c & -276 & -42b & 66c & 276 & -42b & -66c & 102 & -21b & 39c \\
21b & -14b^2 & 0 & 42b & -28b^2 & 0 & -42b & 112b^2 & 0 & -21b & 56b^2 & 0 \\
39c & 0 & 18c^2 & 66c & 0 & -24c^2 & -66c & 0 & 24c^2 & -39c & 0 & -18c^2 \\
-276 & -42b & -66c & -102 & -21b & 39c & 102 & -21b & -39c & 276 & -42b & 66c \\
42b & -28b^2 & 0 & 21b & -14b^2 & 0 & -21b & 56b^2 & 0 & -42b & 112b^2 & 0 \\
-66c & 0 & -24c^2 & -39c & 0 & 18c^2 & 39c & 0 & -18c^2 & 66c & 0 & 24c^2
\end{bmatrix}
\tag{18}
$$

- Based on the discussions for all the three systems considered here, in general the element mass matrix of a nonlocal dynamic system can be expressed as

$$\mathbf{M}_e = \mathbf{M}_{0_e} + \mathbf{M}_{\mu_e} \tag{19}$$

Here $\mathbf{M}_{0_e}$ is the element stiffness matrix corresponding to the underlying local system and $\mathbf{M}_{\mu_e}$ is the additional term arising due to the nonlocal effect.

- The element stiffness matrix remains unchanged.

- Using the finite element formulation, the stiffness matrix of the local and nonlocal system turns out to be identical to each other.
- The mass matrix of the nonlocal system is however different from its equivalent local counterpart.
- Assembling the element matrices and applying the boundary conditions, following the usual procedure of the finite element method one obtains the global mass matrix as

$$\mathbf{M} = \mathbf{M}_0 + \mathbf{M}_\mu \tag{20}$$

- In the above equation $\mathbf{M}_0$ is the usual global mass matrix arising in the conventional local system and $\mathbf{M}_\mu$ is matrix arising due to nonlocal nature of the systems:

$$\mathbf{M}_\mu = \left( \frac{e_0 a}{L} \right)^2 \widehat{\mathbf{M}}_\mu \tag{21}$$

Here $\widehat{\mathbf{M}}_\mu$ is a nonnegative definite matrix. The matrix $\mathbf{M}_\mu$ is therefore, a scale-dependent matrix and its influence reduces if the length of the system $L$ is large compared to the parameter $e_0 a$.

- Majority of the current finite element software and other computational tools do not explicitly consider the nonlocal part of the mass matrix. For the design and analysis of future generation of nano electromechanical systems it is vitally important to consider the nonlocal influence.

- We are interested in understanding the impact of the difference in the mass matrix on the dynamic characteristics of the system. In particular the following questions of fundamental interest have been addressed:
  - Under what condition a nonlocal system possess classical local normal modes?
  - How the vibration modes and frequencies of a nonlocal system can be understood in the light of the results from classical local systems?

- By addressing these questions, it would be possible to extend conventional 'local' elasticity based finite element software to analyse nonlocal systems arising in the modelling of complex nanoscale built-up structures.

- The equation of motion of a discretised nonlocal damped system with $n$ degrees of freedom can be expressed as

$$[\mathbf{M}_0 + \mathbf{M}_\mu]\,\ddot{\mathbf{u}}(t) + \mathbf{C}\dot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) = \mathbf{f}(t) \tag{22}$$

- Here $\mathbf{u}(t) \in \mathbb{R}^n$ is the displacement vector, $\mathbf{f}(t) \in \mathbb{R}^n$ is the forcing vector, $\mathbf{K}, \mathbf{C} \in \mathbb{R}^{n \times n}$ are respectively the global stiffness and the viscous damping matrix.

- In general $\mathbf{M}_0$ and $\mathbf{M}_\mu$ are positive definite symmetric matrices, $\mathbf{C}$ and $\mathbf{K}$ are non-negative definite symmetric matrices. The equation of motion of corresponding local system is given by

$$\mathbf{M}_0\ddot{\mathbf{u}}_0(t) + \mathbf{C}\dot{\mathbf{u}}_0(t) + \mathbf{K}\mathbf{u}_0(t) = \mathbf{f}(t) \tag{23}$$

where $\mathbf{u}_0(t) \in \mathbb{R}^n$ is the local displacement vector.

- The natural frequencies ($\omega_j \in \mathbb{R}$) and the mode shapes ($\mathbf{x}_j \in \mathbb{R}^n$) of the corresponding undamped local system can be obtained by solving the matrix eigenvalue problem [23] as

$$\mathbf{K}\mathbf{x}_j = \omega_j^2\mathbf{M}_0\mathbf{x}_j, \quad \forall j = 1, 2, \ldots, n \tag{24}$$

## Dynamics of the local system

- The undamped local eigenvectors satisfy an orthogonality relationship over the local mass and stiffness matrices, that is

$$\mathbf{x}_k^T \mathbf{M}_0 \mathbf{x}_j = \delta_{kj} \tag{25}$$

$$\text{and} \quad \mathbf{x}_k^T \mathbf{K} \mathbf{x}_j = \omega_j^2 \delta_{kj}, \quad \forall k, j = 1, 2, \ldots, n \tag{26}$$

where $\delta_{kj}$ is the Kroneker delta function. We construct the local modal matrix

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n] \in \mathbb{R}^n \tag{27}$$

- The local modal matrix can be used to diagonalize the local system (23) provided the damping matrix $\mathbf{C}$ is simultaneously diagonalizable with $\mathbf{M}_0$ and $\mathbf{K}$.
- This condition, known as the proportional damping, originally introduced by Lord Rayleigh [27] in 1877, is still in wide use today.
- The mathematical condition for proportional damping can be obtained from the commutitative behaviour of the system matrices [28]. This can be expressed as

$$\mathbf{C}\mathbf{M}_0^{-1}\mathbf{K} = \mathbf{K}\mathbf{M}_0^{-1}\mathbf{C} \tag{28}$$

or equivalently $\mathbf{C} = \mathbf{M}_0 f(\mathbf{M}_0^{-1}\mathbf{K})$ as shown in [29].

- Considering undamped nonlocal system and premultiplying the equation by $\mathbf{M}_0^{-1}$ we have

$$\left(\mathbf{I}_n + \mathbf{M}_0^{-1}\mathbf{M}_\mu\right)\ddot{\mathbf{u}}(t) + \left(\mathbf{M}_0^{-1}\mathbf{K}\right)\mathbf{u}(t) = \mathbf{M}_0^{-1}\mathbf{f}(t) \tag{29}$$

- This system can be diagonalized by a similarity transformation which also diagonalise $\left(\mathbf{M}_0^{-1}\mathbf{K}\right)$ provided the matrices $\left(\mathbf{M}_0^{-1}\mathbf{M}_\mu\right)$ and $\left(\mathbf{M}_0^{-1}\mathbf{K}\right)$ commute. This implies that the condition for existence of classical local normal modes is

$$\left(\mathbf{M}_0^{-1}\mathbf{K}\right)\left(\mathbf{M}_0^{-1}\mathbf{M}_\mu\right) = \left(\mathbf{M}_0^{-1}\mathbf{M}_\mu\right)\left(\mathbf{M}_0^{-1}\mathbf{K}\right) \tag{30}$$

$$\text{or} \quad \mathbf{K}\mathbf{M}_0^{-1}\mathbf{M}_\mu = \mathbf{M}_\mu\mathbf{M}_0^{-1}\mathbf{K} \tag{31}$$

- If the above condition is satisfied, then a nonlocal undamped system can be diagonalised by the classical local normal modes. However, it is also possible to have nonlocal normal modes which can diagonalize the nonlocal undamped system as discussed next.

- Nonlocal normal modes can be obtained by the undamped nonlocal eigenvalue problem

$$\mathbf{K}\mathbf{u}_j = \lambda_j^2 \left[\mathbf{M}_0 + \mathbf{M}_\mu\right]\mathbf{u}_j, \quad \forall j = 1, 2, \ldots, n \tag{32}$$

- Here $\lambda_j$ and $\mathbf{u}_j$ are the nonlocal natural frequencies and nonlocal normal modes of the system. We can define a nonlocal modal matrix

$$\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n] \in \mathbb{R}^n \tag{33}$$

which will unconditionally diagonalize the nonlocal undamped system. It should be remembered that in general nonlocal normal modes and frequencies will be different from their local counterparts.

- Under certain restrictive condition it may be possible to diagonalise the damped nonlocal system using classical normal modes.
- Premultiplying the equation of motion (22) by $\mathbf{M}_0^{-1}$, the required condition is that $\left(\mathbf{M}_0^{-1}\mathbf{M}_\mu\right)$, $\left(\mathbf{M}_0^{-1}\mathbf{C}\right)$ and $\left(\mathbf{M}_0^{-1}\mathbf{K}\right)$ must commute pairwise. This implies that in addition to the two conditions given by Eqs. (28) and (31), we also need a third condition

$$\mathbf{C}\mathbf{M}_0^{-1}\mathbf{M}_\mu = \mathbf{M}_\mu\mathbf{M}_0^{-1}\mathbf{C} \tag{34}$$

- If we consider the diagonalization of the nonlocal system by the nonlocal modal matrix in (33), then the concept of proportional damping can be applied similar to that of the local system. One can obtain the required condition similar to Caughey's condition [28] as in Eq. (28) by replacing the mass matrix with $\mathbf{M}_0 + \mathbf{M}_\mu$. If this condition is satisfied, then the equation of motion can be diagonalised by the nonlocal normal modes and in general not by the classical normal modes.

- Majority of the existing finite element software calculate the classical normal modes.
- However, it was shown that only under certain restrictive condition, the classical normal modes can be used to diagonalise the system.
- In general one need to use nonlocal normal modes to diagonalise the equation of motion (22), which is necessary for efficient dynamic analysis and physical understanding of the system.
- We aim to express nonlocal normal modes in terms of classical normal modes.
- Since the classical normal modes are well understood, this approach will allow us to develop physical understanding of the nonlocal normal modes.

## Projection in the space of undamped classical modes

- For distinct undamped eigenvalues ($\omega_l^2$), local eigenvectors $\mathbf{x}_l$, $\forall l = 1, \ldots, n$, form a complete set of vectors. For this reason each nonlocal normal mode $\mathbf{u}_j$ can be expanded as a linear combination of $\mathbf{x}_l$:

$$\mathbf{u}_j = \sum_{l=1}^{n} \alpha_l^{(j)} \mathbf{x}_l \tag{35}$$

- Without any loss of generality, we can assume that $\alpha_j^{(j)} = 1$ (normalization) which leaves us to determine $\alpha_l^{(j)}, \forall l \neq j$.

- Substituting the expansion of $\mathbf{u}_j$ into the eigenvalue equation (32), one obtains

$$\left[ -\lambda_j^2 \left( \mathbf{M}_0 + \mathbf{M}_\mu \right) + \mathbf{K} \right] \sum_{l=1}^{n} \alpha_l^{(j)} \mathbf{x}_l = \mathbf{0} \tag{36}$$

For the case when $\alpha_l^{(j)}$ are approximate, the error involving the projection in Eq. (35) can be expressed as

$$\varepsilon_j = \sum_{l=1}^{n} \left[ -\lambda_j^2 \left( \mathbf{M}_0 + \mathbf{M}_\mu \right) + \mathbf{K} \right] \alpha_l^{(j)} \mathbf{x}_l \tag{37}$$

- We use a Galerkin approach to minimise this error by viewing the expansion as a projection in the basis functions $\mathbf{x}_l \in \mathbb{R}^n, \forall l = 1, 2, \ldots n$. Therefore, making the error orthogonal to the basis functions one has

$$\varepsilon_j \perp \mathbf{x}_l \quad \text{or} \quad \mathbf{x}_k^T \varepsilon_j = 0 \quad \forall \ k = 1, 2, \ldots, n \tag{38}$$

- Using the orthogonality property of the undamped local modes

$$\sum_{l=1}^{n} \left[ -\lambda_j^2 \left( \delta_{kl} + M'_{\mu_{kl}} \right) + \omega_k^2 \delta_{kl} \right] \alpha_l^{(j)} = 0 \tag{39}$$

where $M'_{\mu_{kl}} = \mathbf{x}_k^T \mathbf{M}_\mu \mathbf{x}_l$ are the elements of the nonlocal part of the modal mass matrix.

- Assuming the off-diagonal terms of the nonlocal part of the modal mass matrix are small and $\alpha_l^{(j)} \ll 1, \forall l \neq j$, approximate nonlocal natural frequencies can be obtained as

$$\lambda_j \approx \frac{\omega_j}{\sqrt{1 + M'_{\mu_{jj}}}} \tag{40}$$

- When $k \neq j$, from Eq. (39) we have

$$\left[-\lambda_j^2 \left(1 + M'_{\mu_{kk}}\right) + \omega_k^2\right] \alpha_k^{(j)} - \lambda_j^2 \sum_{l \neq k}^{n} \left(M'_{\mu_{kl}}\right) \alpha_l^{(j)} = 0 \qquad (41)$$

- Recalling that $\alpha_j^{(j)} = 1$, this equation can be expressed as

$$\left[-\lambda_j^2 \left(1 + M'_{\mu_{kk}}\right) + \omega_k^2\right] \alpha_k^{(j)} = \lambda_j^2 \left[M'_{\mu_{kj}} + \sum_{l \neq k \neq j}^{n} M'_{\mu_{kl}} \alpha_l^{(j)}\right] \qquad (42)$$

- Solving for $\alpha_k^{(j)}$, the nonlocal normal modes can be expressed in terms of the classical normal modes as

$$\mathbf{u}_j \approx \mathbf{x}_j + \sum_{k \neq j}^{n} \frac{\lambda_j^2}{\left(\lambda_k^2 - \lambda_j^2\right)} \frac{M'_{\mu_{kj}}}{\left(1 + M'_{\mu_{kk}}\right)} \mathbf{x}_k \qquad (43)$$

Equations (40) and (43) completely defines the nonlocal natural frequencies and mode shapes in terms of the local natural frequencies and mode shapes. The following insights about the nonlocal normal modes can be deduced

- Each nonlocal mode can be viewed as a sum of two principal components. One of them is parallel to the corresponding local mode and the other is orthogonal to it as all $\mathbf{x}_k$ are orthogonal to $\mathbf{x}_j$ for $j \neq k$.

- Due to the term $\left( \lambda_k^2 - \lambda_j^2 \right)$ in the denominator, for a given nonlocal mode, only few adjacent local modes contributes to the orthogonal component.

- For systems with well separated natural frequencies, the contribution of the orthogonal component becomes smaller compared to the parallel component.

- Taking the Fourier transformation of the equation of motion (22) we have

$$\mathbf{D}(\mathrm{i}\omega)\bar{\mathbf{u}}(\mathrm{i}\omega) = \bar{\mathbf{f}}(\mathrm{i}\omega) \tag{44}$$

where the nonlocal dynamic stiffness matrix is given by

$$\mathbf{D}(\mathrm{i}\omega) = -\omega^2 \left[\mathbf{M}_0 + \mathbf{M}_\mu\right] + \mathrm{i}\omega\mathbf{C} + \mathbf{K} \tag{45}$$

- In Eq. (44) $\bar{\mathbf{u}}(\mathrm{i}\omega)$ and $\bar{\mathbf{f}}(\mathrm{i}\omega)$ are respectively the Fourier transformations of the response and the forcing vectors.
- Using the local modal matrix (27), the dynamic stiffness matrix can be transformed to the modal coordinate as

$$\mathbf{D}'(\mathrm{i}\omega) = \mathbf{X}^T \mathbf{D}(\mathrm{i}\omega)\mathbf{X} = -\omega^2 \left[\mathbf{I} + \mathbf{M}'_\mu\right] + \mathrm{i}\omega\mathbf{C}' + \mathbf{\Omega}^2 \tag{46}$$

where $\mathbf{I}$ is a $n$-dimensional identity matrix, $\mathbf{\Omega}^2$ is a diagonal matrix containing the squared local natural frequencies and $(\bullet)'$ denotes that the quantity is in the modal coordinates.

- We separate the diagonal and off-diagonal terms as

$$\mathbf{D}'(\mathrm{i}\omega) = \underbrace{-\omega^2 \left[\mathbf{I} + \overline{\mathbf{M}}'_\mu\right] + \mathrm{i}\omega\overline{\mathbf{C}}' + \mathbf{\Omega}^2}_{\text{diagonal}} + \underbrace{\left(-\omega^2\Delta\mathbf{M}'_\mu + \mathrm{i}\omega\Delta\mathbf{C}'\right)}_{\text{off-diagonal}} \qquad (47)$$

$$= \overline{\mathbf{D}}'(\mathrm{i}\omega) + \Delta\mathbf{D}'(\mathrm{i}\omega) \qquad (48)$$

- The dynamic response of the system can be obtained as

$$\bar{\mathbf{u}}(\mathrm{i}\omega) = \mathbf{H}(\mathrm{i}\omega)\bar{\mathbf{f}}(\mathrm{i}\omega) = \left[\mathbf{X}\mathbf{D}'^{-1}(\mathrm{i}\omega)\mathbf{X}^T\right]\bar{\mathbf{f}}(\mathrm{i}\omega) \qquad (49)$$

  where the matrix $\mathbf{H}(\mathrm{i}\omega)$ is known as the transfer function matrix.
- From the expression of the modal dynamic stiffness matrix we have

$$\mathbf{D}'^{-1}(\mathrm{i}\omega) = \left[\overline{\mathbf{D}}'(\mathrm{i}\omega)\left(\mathbf{I} + \overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega)\Delta\mathbf{D}'(\mathrm{i}\omega)\right)\right]^{-1} \qquad (50)$$

$$\approx \overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega) - \overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega)\Delta\mathbf{D}'(\mathrm{i}\omega)\overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega) \qquad (51)$$

- Substituting the approximate expression of $\mathbf{D}^{'^{-1}}(\mathrm{i}\omega)$ from Eq. (51) into the expression of the transfer function matrix in Eq. (49) we have

$$\mathbf{H}(\mathrm{i}\omega) = \left[\mathbf{X}\mathbf{D}^{'^{-1}}(\mathrm{i}\omega)\mathbf{X}^T\right] \approx \overline{\mathbf{H}}'(\mathrm{i}\omega) - \Delta\mathbf{H}'(\mathrm{i}\omega) \tag{52}$$

where

$$\overline{\mathbf{H}}'(\mathrm{i}\omega) = \mathbf{X}\overline{\mathbf{D}}'(\mathrm{i}\omega)\mathbf{X}^T = \sum_{k=1}^{n} \frac{\mathbf{x}_k\mathbf{x}_k^T}{-\omega^2\left(1 + M'_{\mu_{kk}}\right) + 2\mathrm{i}\omega\omega_k\zeta_k + \omega_k^2} \tag{53}$$

$$\text{and} \quad \Delta\mathbf{H}'(\mathrm{i}\omega) = \mathbf{X}\overline{\mathbf{D}}^{'^{-1}}(\mathrm{i}\omega)\Delta\mathbf{D}'(\mathrm{i}\omega)\overline{\mathbf{D}}^{'^{-1}}(\mathrm{i}\omega)\mathbf{X}^T \tag{54}$$

- Equation (52) therefore completely defines the transfer function of the damped nonlocal system in terms of the classical normal modes. This can be useful in practice as all the quantities arise in this expression can be obtained from a conventional finite element software. One only needs the nonlocal part of the mass matrix as derived in 2.

Some notable features of the expression of the transfer function matrix are

- For lightly damped systems, the transfer function will have peaks around the nonlocal natural frequencies derived previously.

- The error in the transfer function depends on two components. They include the off-diagonal part of the of the modal nonlocal mass matrix $\triangle \mathbf{M}'_\mu$ and the off-diagonal part of the of the modal damping matrix $\triangle \mathbf{C}'$. While the error in in the damping term is present for non proportionally damped local systems, the error due to the nonlocal modal mass matrix in unique to the nonlocal system.

- For a proportionally damped system $\triangle \mathbf{C}' = \mathbf{O}$. For this case error in the transfer function only depends on $\triangle \mathbf{M}'_\mu$.

- In general, error in the transfer function is expected to be higher for higher frequencies as both $\triangle \mathbf{C}'$ and $\triangle \mathbf{M}'_\mu$ are weighted by frequency $\omega$.

The expressions of the nonlocal natural frequencies (40), nonlocal normal modes (43) and the nonlocal transfer function matrix (52) allow us to understand the dynamic characteristic of a nonlocal system in a qualitative and quantitative manner in the light of equivalent local systems.

**Figure :** Axial vibration of a zigzag (7, 0) single-walled carbon nanotube (SWCNT) with clamped-free boundary condition.

## Axial vibration of a single-walled carbon nanotube

- A single-walled carbon nanotube (SWCNT) is considered.
- A zigzag (7, 0) SWCNT with Young's modulus $E = 6.85$ TPa, $L = 25$nm, density $\rho = 9.517 \times 10^3$ kg/m$^3$ and thickness $t = 0.08$nm is used
- For a carbon nanotube with chirality $(n_i, m_i)$, the diameter can be given by

$$d_i = \frac{r}{\pi}\sqrt{n_i^2 + m_i^2 + n_i m_i} \qquad (55)$$

  where $r = 0.246$nm. The diameter of the SWCNT shown in 7 is 0.55nm.
- A constant modal damping factor of 1% for all the modes is assumed.
- We consider clamped-free boundary condition for the SWCNT. Undamped nonlocal natural frequencies can be obtained as

$$\lambda_j = \sqrt{\frac{EA}{m}} \frac{\sigma_j}{\sqrt{1 + \sigma_j^2(e_0 a)^2}}, \quad \text{where} \quad \sigma_j = \frac{(2j-1)\pi}{2L}, \quad j = 1, 2, \cdots \ (56)$$

  $EA$ is the axial rigidity and $m$ is the mass per unit length of the SWCNT.
- For the finite element analysis the SWCNT is divided into 200 elements. The dimension of each of the system matrices become $200 \times 200$, that is $n = 200$.
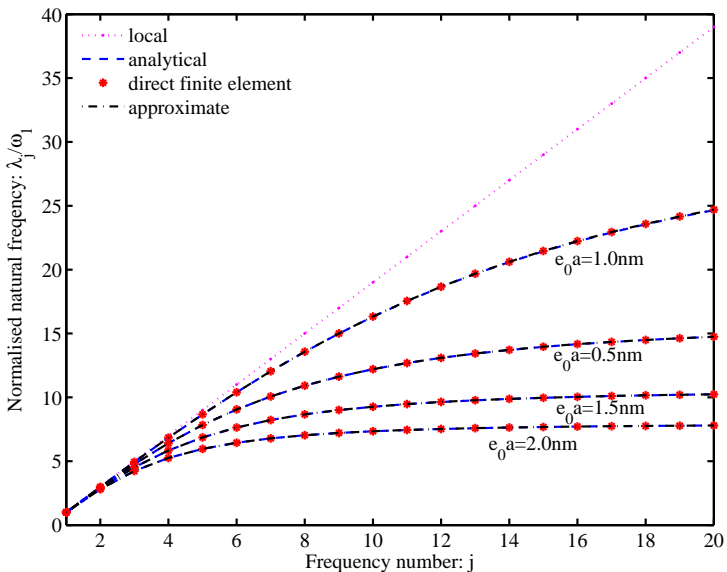
First 20 undamped natural frequencies for the axial vibration of SWCNT.
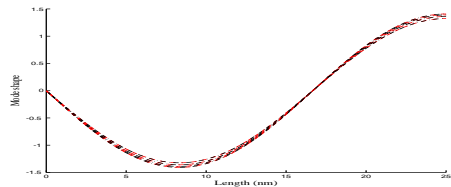
(a) Mode 2
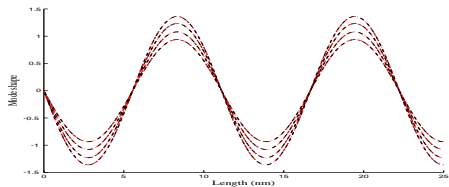
(b) Mode 5
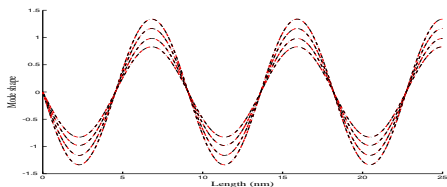
(c) Mode 6
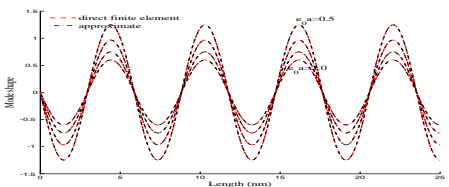
(d) Mode 9

**Figure :** Four selected mode shapes for the axial vibration of SWCNT. Exact finite element results are compared with the approximate analysis based on local eigensolutions. In each subplot four different values of $e_0a$, namely 0.5, 1.0, 1.5 and 2.0nm have been used.
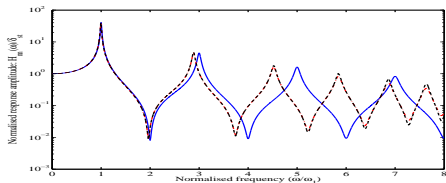
(a) $e_0 a = 0.5$nm

(b) $e_0 a = 1.0$nm

(c) $e_0 a = 1.5$nm

(d) $e_0 a = 2.0$nm

**Figure :** Amplitude of the normalised frequency response of the SWCNT at the tip for different values of $e_0 a$. Exact finite element results are compared with the approximate analysis based on local eigensolutions.

**Transverse vibration of a single-layer graphene sheet**

- A rectangular single-layer graphene sheet (SLGS) is considered to examine the transverse vibration characteristics of nanoplates.
- The graphene sheet is of dimension *L*=20nm, *W*=15nm and Young's modulus $E = 1.0$ TPa, density $\rho = 2.25 \times 10^3$ kg/m$^3$, Poisson's ratio $\nu = 0.3$ and thickness *h* = 0.34nm is considered
- We consider simply supported boundary condition along the four edges for the SLGS. Undamped nonlocal natural frequencies are

$$\lambda_{ij} = \sqrt{\frac{D}{m}} \frac{\beta_{ij}^2}{\sqrt{1 + \beta_{ij}^2(e_0 a)^2}} \quad \text{where} \quad \beta_{ij} = \sqrt{(i\pi/L)^2 + (j\pi/W)^2}, \ i,j = 1,2,\cdots$$

(57)

*D* is the bending rigidity and *m* is the mass per unit area of the SLGS.

- For the finite element analysis the DWCNT is divided into $20 \times 15$ elements. The dimension of each of the system matrices become $868 \times 868$, that is $n = 868$.
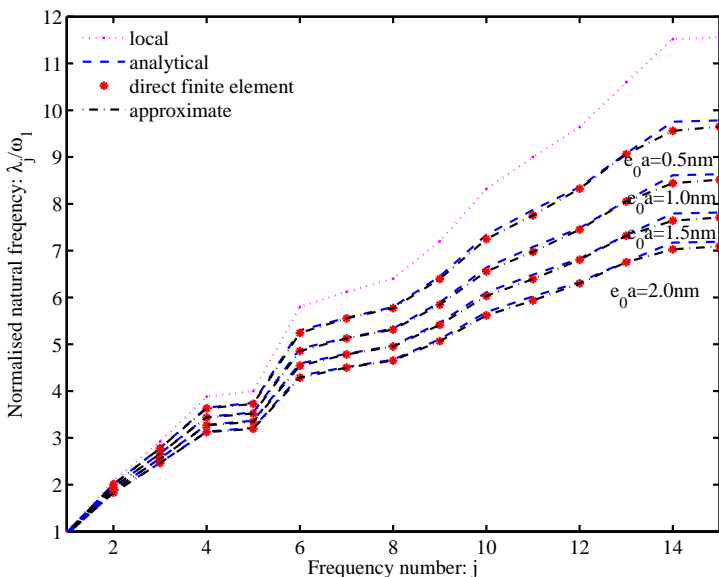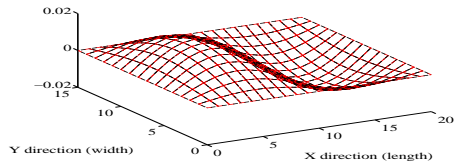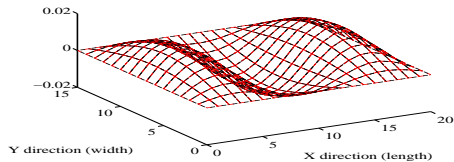
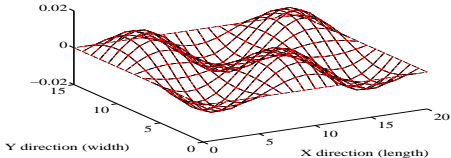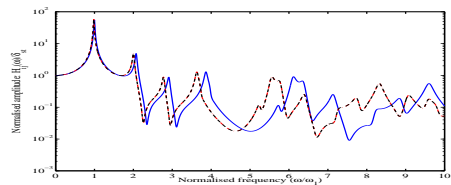First 15 undamped natural frequencies for the transverse vibration of SLGS.
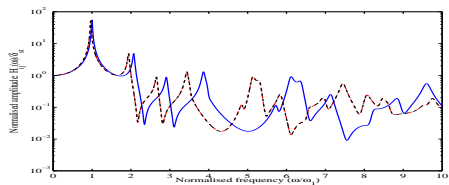
(a) Mode 2

(b) Mode 4
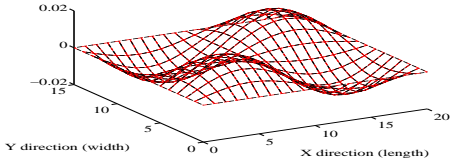
(c) Mode 5

(d) Mode 6

**Figure :** Four selected mode shapes for the transverse vibration of SLGS for $e_0 a = 2$nm. Exact finite element results (solid line)are compared with the approximate analysis based on local eigensolutions (dashed line).

(a) $e_0 a = 0.5$nm

(b) $e_0 a = 1.0$nm
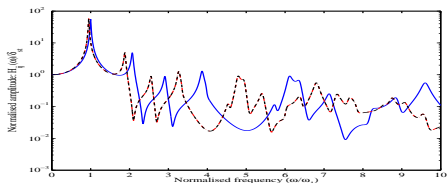
(c) $e_0 a = 1.5$nm

(d) $e_0 a = 2.0$nm

**Figure :** Amplitude of the normalised frequency response $H_{ij}(\omega)$ for $i = 475, j = 342$ of the SLGS for different values of $e_0 a$. Exact finite element results are compared with the approximate analysis based on local eigensolutions.
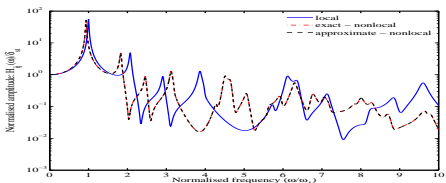
- Nonlocal elasticity is a promising theory for the modelling of nanoscale dynamical systems such as carbon nantotubes and graphene sheets.
- The mass matrix can be decomposed into two parts, namely the classical local mass matrix $\mathbf{M}_0$ and a nonlocal part denoted by $\mathbf{M}_\mu$. The nonlocal part of the mass matrix is scale-dependent and vanishes for systems with large length-scale.
- An undamped nonlocal system will have classical normal modes provided the nonlocal part of the mass matrix satisfy the condition $\mathbf{K}\mathbf{M}_0^{-1}\mathbf{M}_\mu = \mathbf{M}_\mu\mathbf{M}_0^{-1}\mathbf{K}$ where $\mathbf{K}$ is the stiffness matrix.
- A viscously damped nonlocal system with damping matrix $\mathbf{C}$ will have classical normal modes provided $\mathbf{C}\mathbf{M}_0^{-1}\mathbf{K} = \mathbf{K}\mathbf{M}_0^{-1}\mathbf{C}$ and $\mathbf{C}\mathbf{M}_0^{-1}\mathbf{M}_\mu = \mathbf{M}_\mu\mathbf{M}_0^{-1}\mathbf{C}$ in addition to the previous condition.

- Natural frequency of a general nonlocal system can be expressed as $\lambda_j \approx \frac{\omega_j}{\sqrt{1+M'_{\mu_{jj}}}}, \forall j = 1, 2, \cdots$ where $\omega_j$ are the corresponding local frequencies and $M'_{\mu_{jj}}$ are the elements of nonlocal part of the mass matrix in the modal coordinate.

- Every nonlocal normal mode can be expressed as a sum of two principal components as $\mathbf{u}_j \approx \mathbf{x}_j + \left( \sum_{k \neq j}^n \frac{\lambda_j^2}{\left(\lambda_k^2 - \lambda_j^2\right)} \frac{M'_{\mu_{kj}}}{\left(1+M'_{\mu_{kk}}\right)} \mathbf{x}_k \right), \forall j = 1, 2, \cdots$. One of them is parallel to the corresponding local mode $\mathbf{x}_j$ and the other is orthogonal to it.

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