Nonlocal dynamics of nanoscale structures: Part 1

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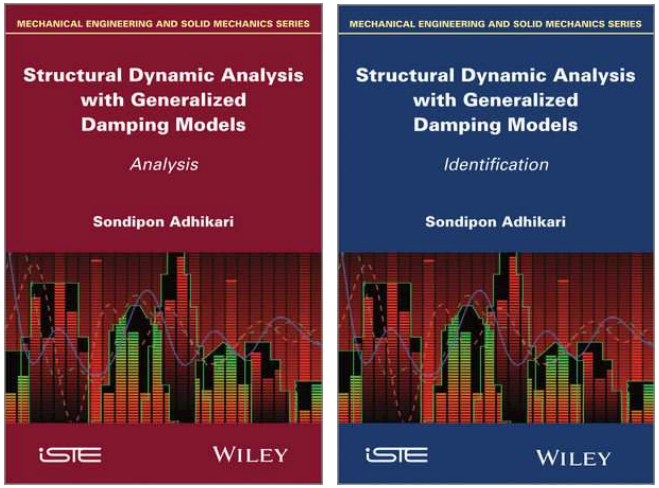
My research interests

- *Development* of fundamental computational methods for structural dynamics and uncertainty quantification

  A. Dynamics of complex systems



  B. Inverse problems for linear and non-linear dynamics

  C. Uncertainty quantification in computational mechanics

- *Applications* of computational mechanics to emerging multidisciplinary research areas

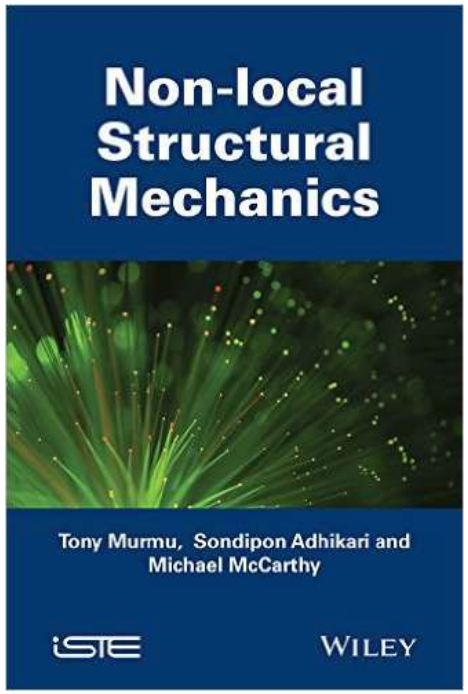
  D. Vibration energy harvesting / dynamics of wind turbines

  E. Computational nanomechanics

Text book for the course

The main text book for the course is:

- Karličić, D. Murmu, T., Adhikari, S. and McCarthy, M., **Non-local Structural Mechanics**, Wiley-ISTE, 2015 (Hardback 354 pp., ISBN: 1848215223).



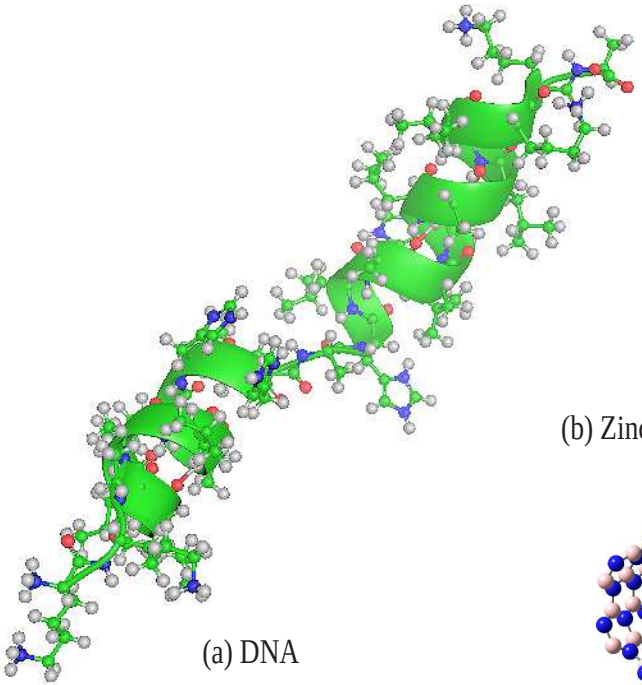
Outline of this talk

1. **Introduction**
2. **Overview of nonlocal continuum mechanics**
3. **Non-local dynamics of elastic rods**
4. **Non-local dynamics of elastic beams**
5. **Non-local dynamics of elastic plates**
6. **Finite element modelling of nonlocal dynamic systems**
   - Axial vibration of nanorods
   - Bending vibration of nanobeams
   - Transverse vibration of nanoplates
7. **Modal analysis of nonlocal dynamical systems**
   - Conditions for classical normal modes
   - Nonlocal normal modes
   - Approximate nonlocal normal modes
8. **Dynamics of damped nonlocal systems**
9. **Numerical illustrations**
   - Axial vibration of a single-walled carbon nanotube
   - Bending vibration of a double-walled carbon nanotube
   - Transverse vibration of a single-layer graphene sheet
10. **Conclusions**

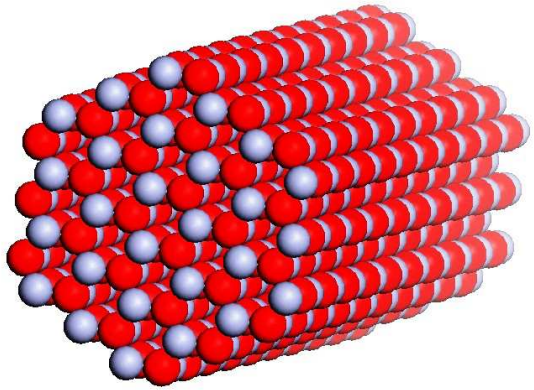
Nanoscale systems

- 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.

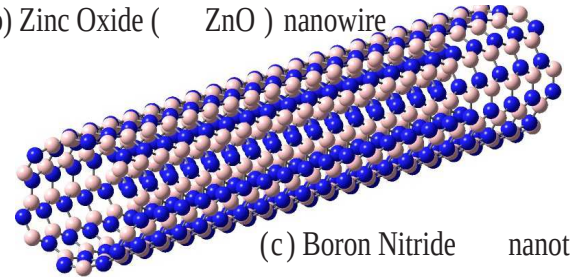
Nanoscale systems



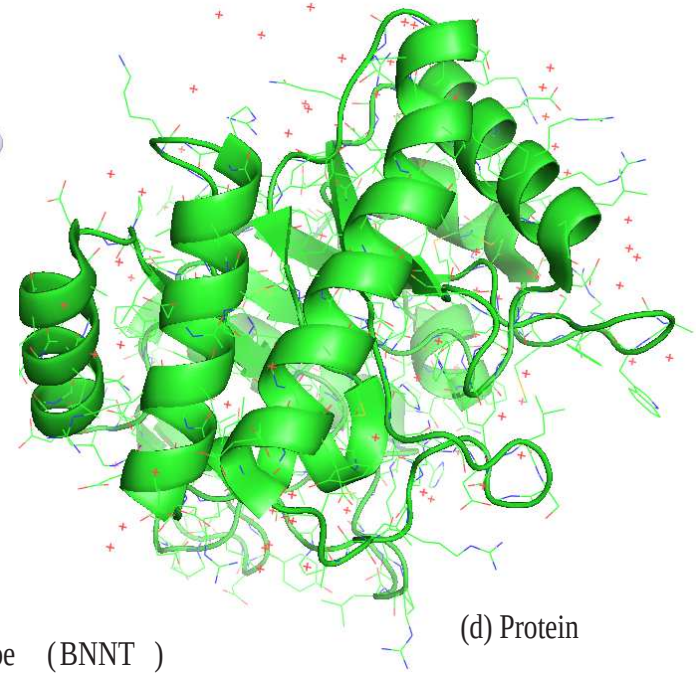
(a) DNA



(b) Zinc Oxide (ZnO) nanowire

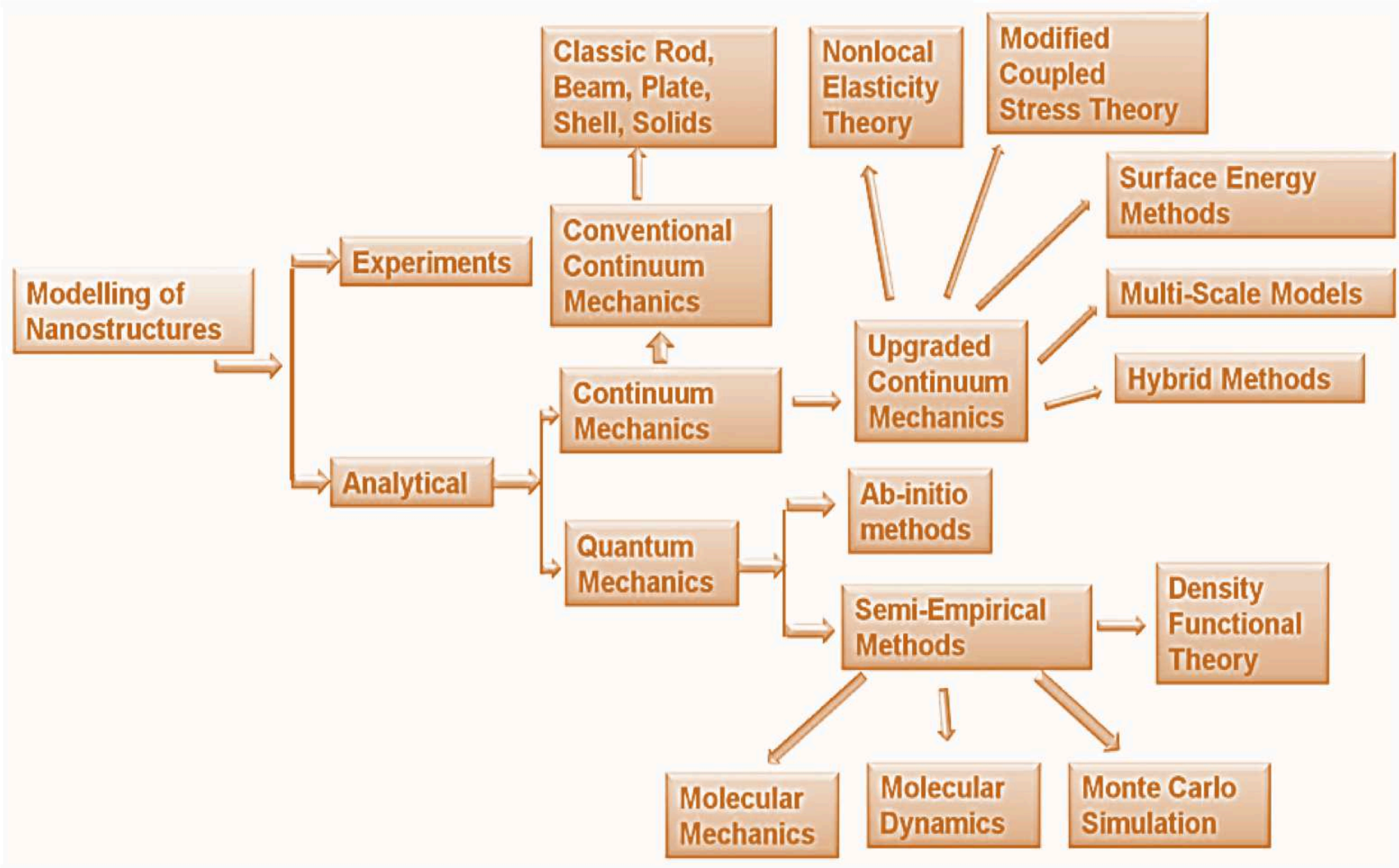


(c) Boron Nitride nanotube (BNNT)

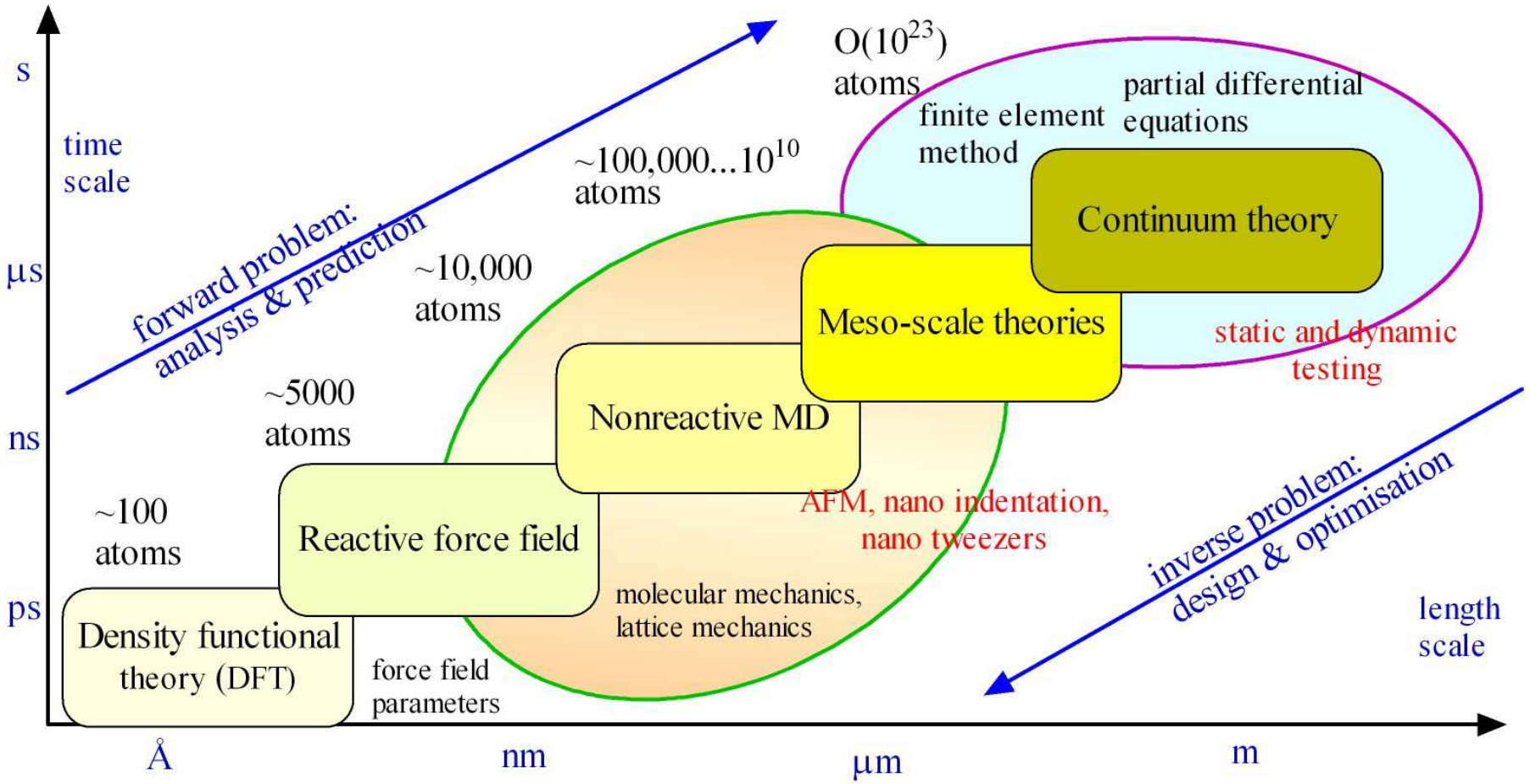


(d) Protein

General approaches for studying nanostructures



Simulation methods



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, according to Eringen [10], 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.
- 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.

Nonlocal continuum mechanics

- The basic equations for nonlocal anisotropic linear homogenous nonlocal elastic body neglecting the body force can be expresses as

$$\begin{aligned} \sigma_{ij,j} &= 0, \\ \sigma_{ij}(\mathbf{x}) &= \int_V \phi(|\mathbf{x}-\mathbf{x}'|,\alpha)\mathbf{t}_{ij}d\mathbf{V}(\mathbf{x}'), \quad \forall x \in \mathbf{V} \\ \mathbf{t}_{ij} &= H_{ijkl}\epsilon_{kl}, \\ \epsilon_{ij} &= 1/2(u_{i,j}+u_{j,i} \end{aligned} \tag{1}$$

- The terms σ_{ij}, t_{ij}, ϵ_{kl} and H_{ijkl} are the nonlocal stress, classical stress, classical strain and fourth order elasticity tensors respectively. The volume integral is over the region **V** occupied by the body. Equation (1) couples the stress due to nonlocal elasticity and the stress due to classical elasticity.
- The kernel function $\phi(|\mathbf{x}-\mathbf{x}'|,\alpha)$ is the nonlocal modulus. The nonlocal modulus acts as an attenuation function incorporating into constitutive equations the nonlocal effects at the reference point **x** produced by local strain at the source $\mathbf{x}'$.

Nonlocal continuum mechanics

- The term $|\mathbf{x} - \mathbf{x}'|$ represents the distance in the Euclidean form and α is a material constant that depends on the internal (e.g. lattice parameter, granular size, distance between the C-C bonds) and external characteristics lengths (e.g. crack length, wave length).
- Material constant α is defined as $\alpha = (e_0 a)/l$ Here e_0 is a constant for calibrating the model with experimental results and other validated models. The parameter e_0 is estimated such that the relations of the nonlocal elasticity model could provide satisfactory approximation to the atomic dispersion curves of the plane waves with those obtained from the atomistic lattice dynamics.
- The terms a and l are the internal (e.g. lattice parameter, granular size, distance between C-C bonds) and external characteristics lengths (e.g. crack length, wave length) of the nanostructure. Equation (1) effectively shows that in nonlocal theory, the stress at a point is a function of the strains at all points in the domain. The classical elasticity can be viewed as a special cade when the kernel function becomes a Dirac delta function.

Nonlocal continuum mechanics

- The direct use of equation (1) in boundary value problems results in integro-partial differential equations and they are generally difficult to solve analytically.
- For this reason, a differential form of nonlocal elasticity equation is often beneficial. According to Eringen [10], this can be achieved for a special case of the kernel function given by

$$\phi(|x - x'|, \alpha) = (2\pi\ell^2\alpha^2)K_0(\sqrt{x \bullet x}/\ell\alpha) \tag{2}$$

- Here K_0 is the modified Bessel function. The equation of motion in terms of nonlocal elasticity can be expressed as

$$\sigma_{ij,j} + f_i = \rho\ddot{u}_i \tag{3}$$

where f_i, ρ and u_i are the components of the body forces, mass density, and the displacement vector, respectively.

Nonlocal continuum mechanics

- The terms i, j takes up the symbols x, y, and z. The operator $(\ddot{\bullet})$ denotes double derivative with respect to time. Assuming the kernel function ϕ as the Green's function, Eringen [10] proposed a differential form of the nonlocal constitutive relation as

$$\sigma_{ij,j} + \mathcal{L}(f_i - \rho \ddot{u}_i) = 0 \tag{4}$$

where

$$\mathcal{L}(\bullet) = [1 - (e_0 a)^2 \nabla^2](\bullet) \tag{5}$$

and ∇^2 is the Laplacian.

- Using this equation the nonlocal constitutive stress-strain relation can be simplified as

$$(1 - \alpha^2 l^2 \nabla^2)\sigma_{ij} = t_{ij} \tag{6}$$

One can use this relationship and derive the equation of motion using conventional variational principle. In the next subsections we consider the dynamics of nonlocal road, beam and plate using this approach.

Nonlocal continuum mechanics

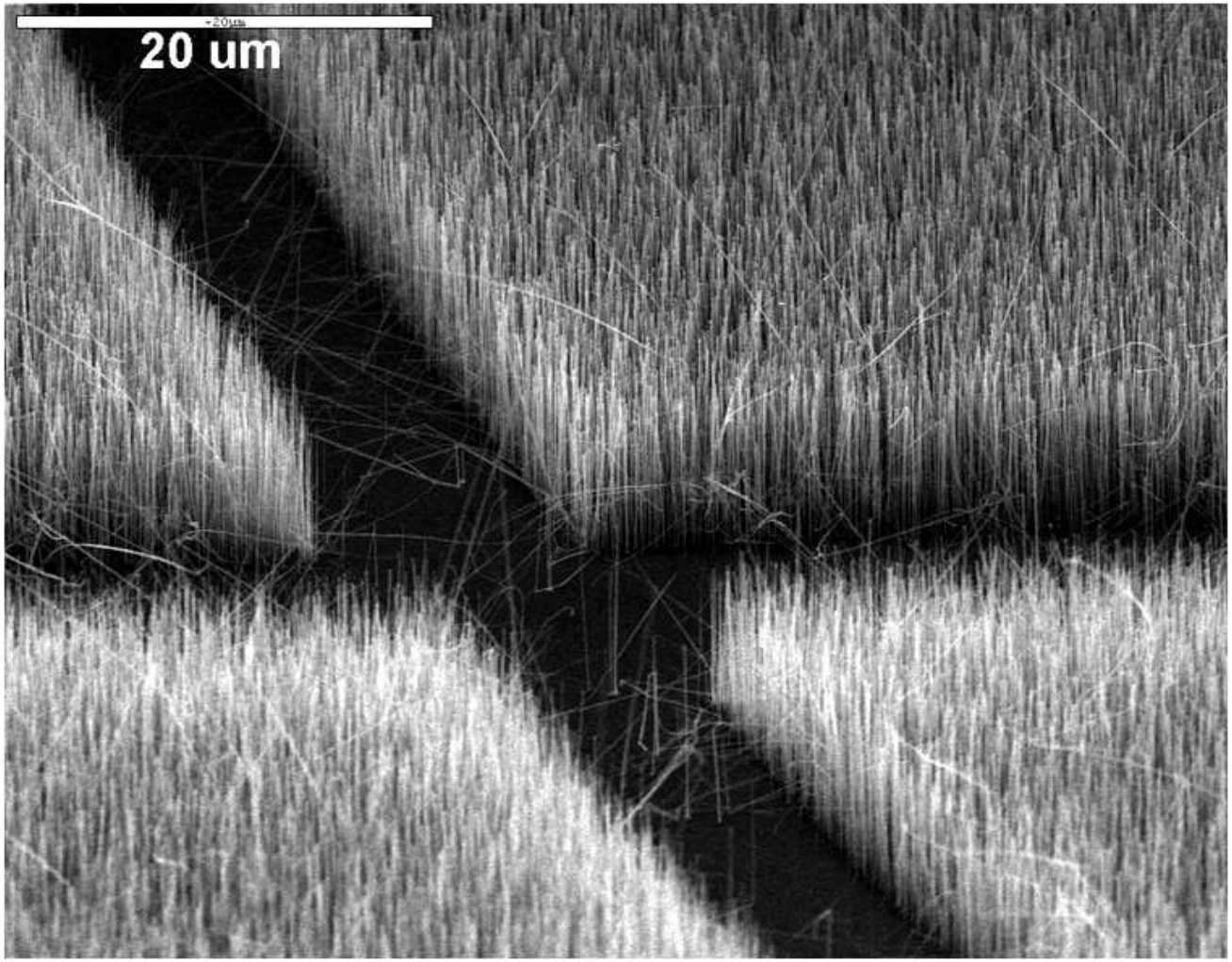
Nonlocal Parameters	Magnitudes	Researchers
a	0.142 nm	(Sudak, 2003)
e_0	0.39	(Eringen, 1983)
	0.288	(Wang and Hu, 2005)
	0-19	(Duan et al., 2007)
$e_0 a$	0.7 nm	(Wang et al, 2008)
	0-2 nm	(Duan and Wang, 2007)
	<2.1 nm	(Wang, 2005)
$e_0 a/l$	0-0.8	(Lu et al., 2006)

Values of nonlocal parameters used in literature.

One-dimensional nanostructures

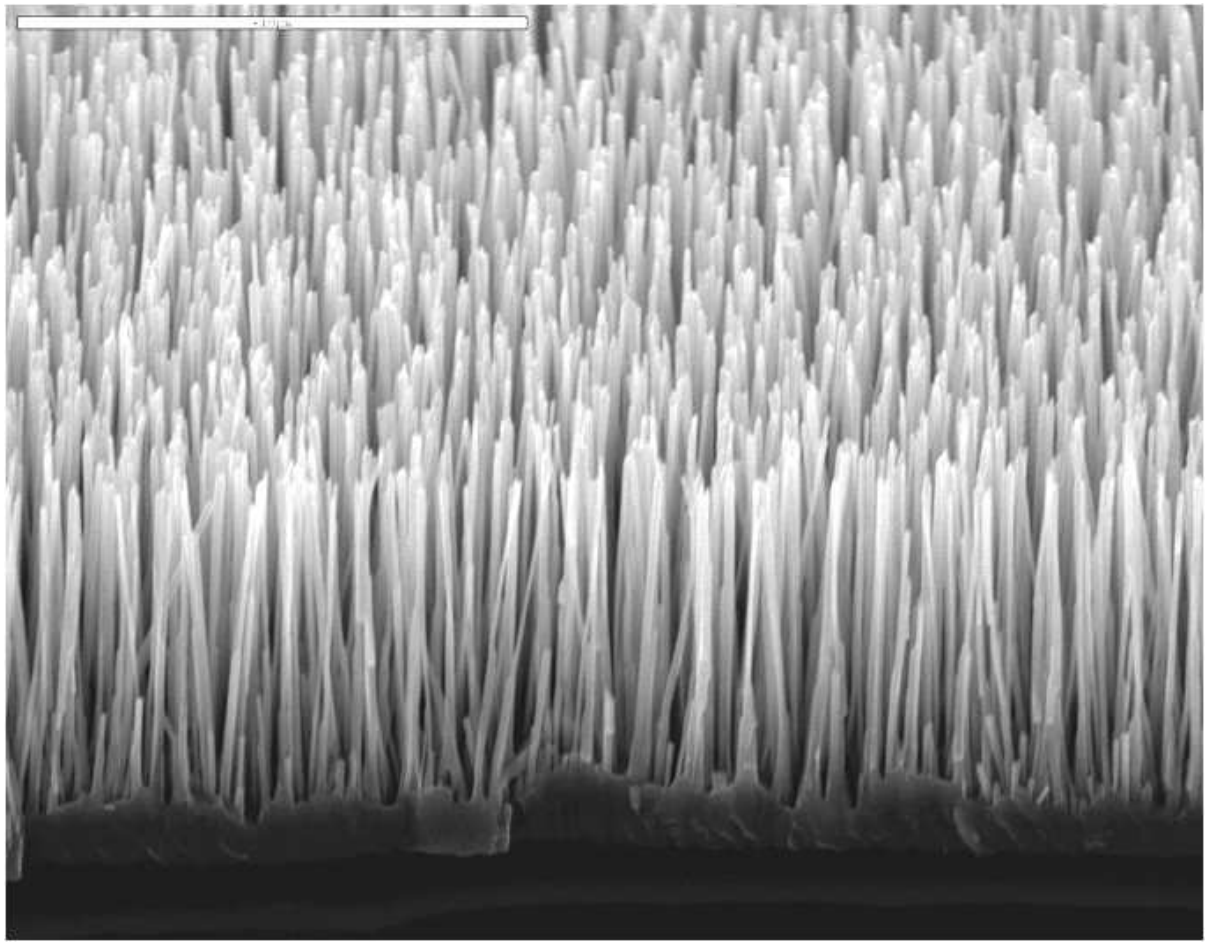
- Recently, various one-dimensional nanostructures have been realized. They include nanodots, nanorods, nanowires, nanobelts, nanotubes, nanobridges and nanonails, nanowalls, nanohelixes, seamless nanorings.
- Among them, one-dimensional nanostructures such as nanotubes, nanorods and nanowires are widely studied. The main reason for this is their simple material formation and device application.
- Nanorods are one-dimensional nanostructures whose lengths are in the range of 1 to 3000 nm.
- These miniscule structures in the form of nanorods or nanowires can be grown using various methods. The popular methods include (i) vapour phase synthesis, (ii) metal-organic chemical vapour deposition, (iii) hydrothermal synthesis.
- Nanorods have found applications in a variety of nanodevices. These include ultraviolet photodetectors, nanosensors, transistors, diodes, LED arrays, etc.

Example: Zinc Oxide (ZnO) nano wires



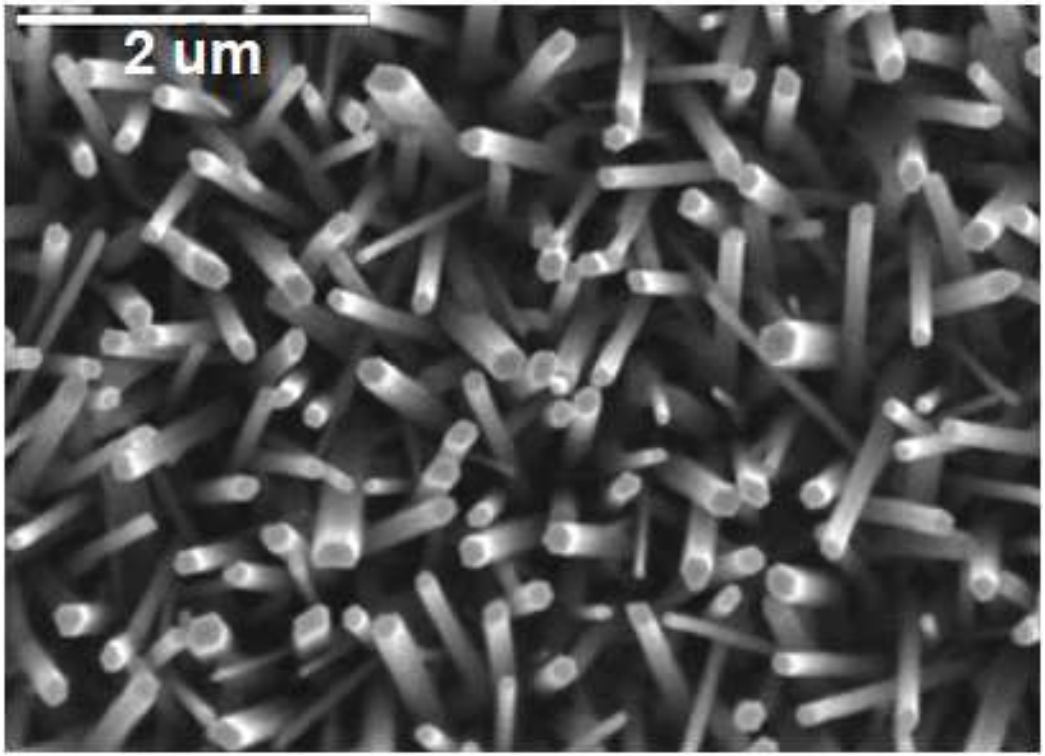
A collection of vertically grown ZnO NWs.

Example: Zinc Oxide (ZnO) nano wires

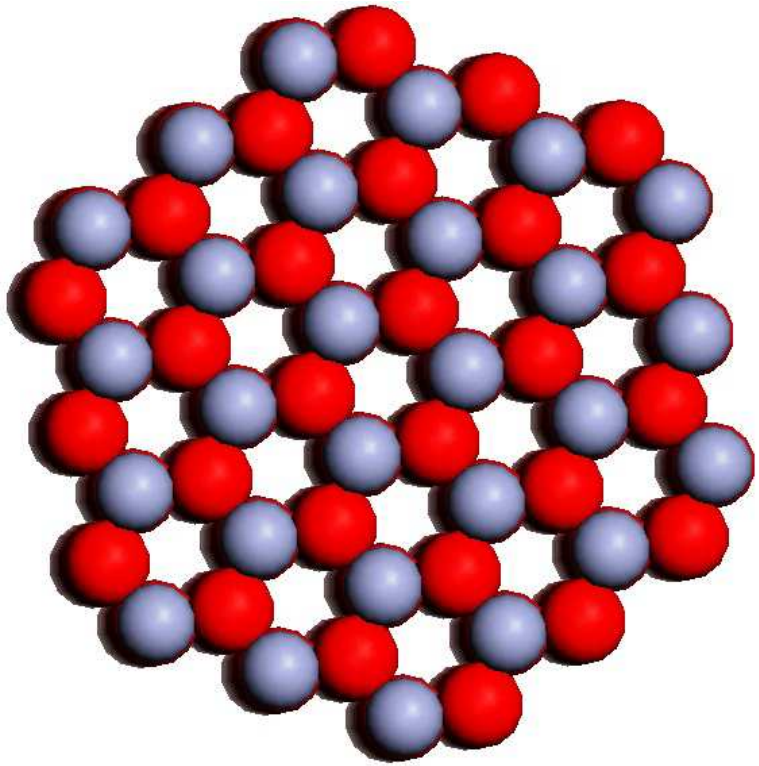


A collection of vertically grown ZnO NWs - close up view.

Example: Zinc Oxide (ZnO) nano wires



(a) The SEM image of a collection of ZnO NW showing hexagonal cross sectional area.



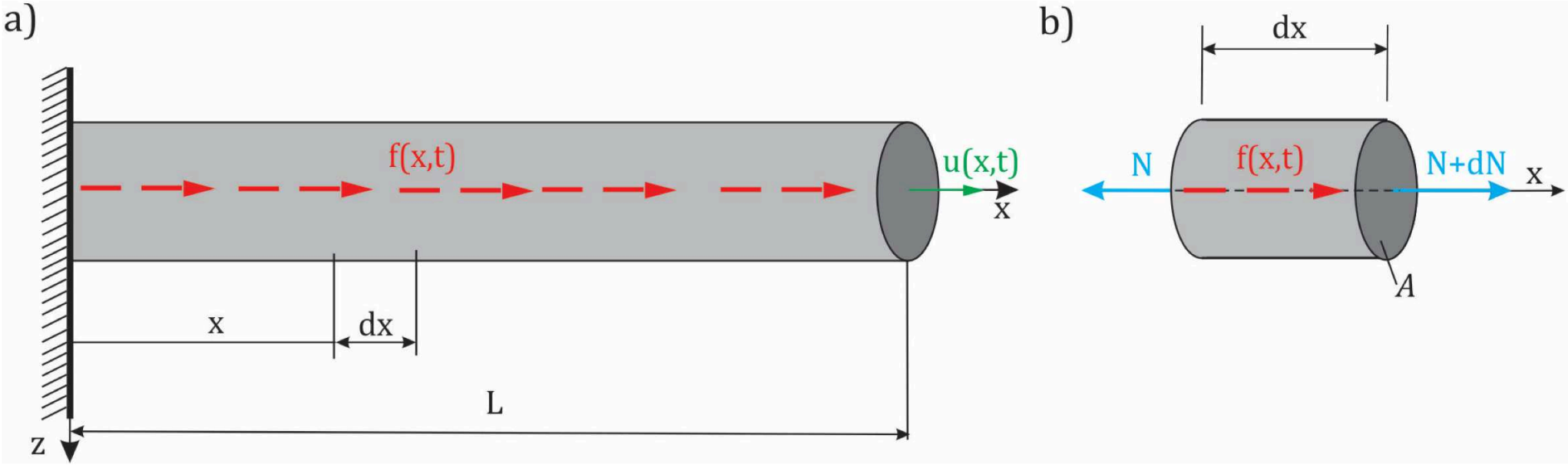
(b) The atomic structure of the cross section of a ZnO NW (the red is O_2 and the grey is Zn atom)

Axial vibration of nanorods

- We will analyze the longitudinal vibration behavior of a single nanorod, based on the nonlocal elasticity theory.
- By using the D? Alembert?s principle, the governing equation of motion is derived and then solved by using the method of separation of variables.
- Two types of boundary conditions are considered for the nanorod, Clamped-Clamped and Clamped?Free.
- The solutions for natural frequencies are obtained analytically in the exact form.

Governing equation of motion of a nanorod

- Consider the equilibrium of an infinitesimal element of the length dx. On the left side of the differential element, we take that the axial force N is the resultant of the normal stress σ_{xx} acting internally on the cross sectional area A.
- On the right end of the differential element, we have the force $N + dN$.



(a) Mechanical model of the longitudinal vibration of a nanorod; b) differential element with corresponding axial stress resultants.

Governing equation of motion of a nanorod

- By applying the D'Alembert's principle, the sum of all forces with respect to x-axes yields

$$-N + (N + dN) + f(x,t)dx = \rho A\, dx\, \frac{\partial^2 u}{\partial t^2} \tag{7}$$

where $dN = \frac{\partial N}{\partial x} dx$ is the differential part of the axial stress resultant N, $u = u(x,t)$ is the axial displacement in the x-direction.

- After some transformations of the above equation, the equilibrium equations are given in the form

$$\frac{dN}{dx} + f(x,t) = \rho A \frac{\partial^2 u}{\partial t^2} \tag{8}$$

in which N is the stress resultant defined as

$$N = \int_A \sigma_{xx}\, dA \tag{9}$$

where term σ_{xx} represents the normal stress in the infinitesimal element of a nanorod.

Governing equation of motion of a nanorod

- According to the nonlocal elasticity theory for one-dimensional case, we get the constitutive relation for a nonlocal elastic body in the differential form as

$$\sigma_{xx} - (e_0 a)^2 \frac{\partial^2 \sigma_{xx}}{\partial x^2} = E\epsilon_{xx} \tag{10}$$

  where the term $(e_0 a)$ denotes the nonlocal parameter and $\epsilon_{xx} = \frac{\partial u}{\partial x}$ denotes the axial strain. The term E is the conventional Young's modulus of the nanostructure component.

- Combining the two preceding equations, the axial stress resultant for the nonlocal theory is obtained as

$$N - (e_0 a)^2 \frac{\partial^2 N}{\partial x^2} = EA\frac{\partial u}{\partial x} \tag{11}$$

  where A is the cross-section defined as $A = \int_A dA$

Governing equation of motion of a nanorod

- The governing equation of motion can be expressed in terms of the axial displacement for the nonlocal elastic constitutive relation. Introducing Eq. (8) into Eq. (15) we obtain the following equation of motion

$$\rho A\frac{\partial^2 u}{\partial t^2} - f(x,t) - EA\frac{\partial^2 u}{\partial x^2} = (e_0 a)^2 \frac{\partial^2}{\partial x^2}\left(\rho A\frac{\partial^2 u}{\partial t^2} - f(x,t)\right) \tag{12}$$

- We utilise Eq. (12) for the development of a mathematical model for the free longitudinal vibration of a nonlocal nanorod. For free vibration, external load is considered to be 0
- Two types of boundary conditions are employed,

Boundary conditions

- *Clamped-Clamped:*

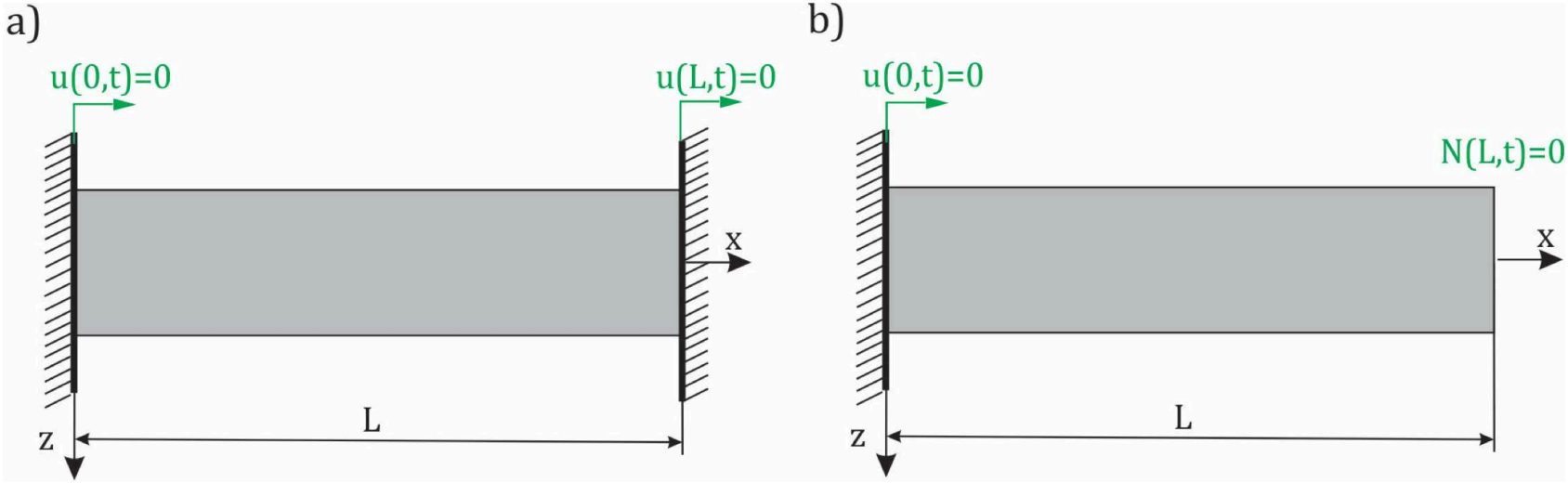
$$u(0,t) = u(L,t) = 0 \tag{13}$$

- *Clamped-Free:*

$$u(0,t) = N(L,t) = 0 \tag{14}$$

where is the nonlocal axial force at the end of a nanorod. From (8) and Eq. (15) we get

$$N(x,t) = (e_0 a)^2 \frac{\partial^2 N}{\partial x^2} + EA\frac{\partial u}{\partial x} \tag{15}$$



Boundary conditions for the longitudinal vibration of a nanorod, a) Clamped-Clamped and b) Clamped-Free.

Free vibration of nano-rods

- Assuming the harmonic motion and applying the method of separation of variables, the solution of Eq. (12) takes the form

$$u(x,t) = \sum_{n=1}^{\infty} X_n(x) T_n(t) \tag{16}$$

where $T_N(t) = \exp(\mathrm{i}\omega_n t)$ is the time function and $X_n(x)$ is the corresponding mode shape function, which depends on the boundary conditions of the system.

- Introducing this solution into Eq. (12) and neglecting the load, one gets the ordinary differential equation for the corresponding mode shape function of the nanorod

$$\frac{d^2 X_n(x)}{dx^2} + \alpha_n^2 X_n(x) = 0 \tag{17}$$

- Here α_n denotes the characteristic values determined from the corresponding boundary conditions as

$$\alpha_n^2 = \frac{\omega_n^2}{E/\rho - (e_0 a)^2 \omega_n^2} \tag{18}$$

Free vibration of nano-rods

- General solution of the mode shapes can be expressed as

$$X_n(x) = A_n \sin \alpha_n x + B_n \cos \alpha_n x \tag{19}$$

where the unknown the constants A_n, B_n should be obtained using the boundary conditions.

- For the *Clamped-Clamped* boundary conditions

$$\sin \alpha_n L = 0 \tag{20}$$

the roots are

$$\alpha_n L = n\pi, \quad n = 1, 2, 3, \cdots, \infty \tag{21}$$

with the corresponding mode shape function as

$$X_n(x) = A_n \sin \alpha_n x = A_n \sin \frac{n\pi}{L} x \tag{22}$$

Free vibration of nano-rods

- For the *Clamped-Free* boundary conditions

$$\cos \alpha_n L = 0 \tag{23}$$

the roots are

$$\alpha_n L = \frac{(2n-1)\pi}{2}, \quad n = 1, 2, 3, \cdots, \infty \tag{24}$$

with the corresponding mode shape function as

$$X_n(x) = A_n \sin \alpha_n x = A_n \sin \frac{(2n-1)\pi}{2L} x \tag{25}$$

- We can obtain nonlocal natural frequencies for the longitudinal vibration of a nanorod from expression and corresponding boundary conditions as

$$\omega_n = \alpha_n \sqrt{\frac{E}{\rho \left(1 + (e_0 a)^2 \alpha_n^2\right)}} \tag{26}$$

where α_n is already defined for the Clamped-Clamped and Clamped-Free boundary conditions.

Numerical results

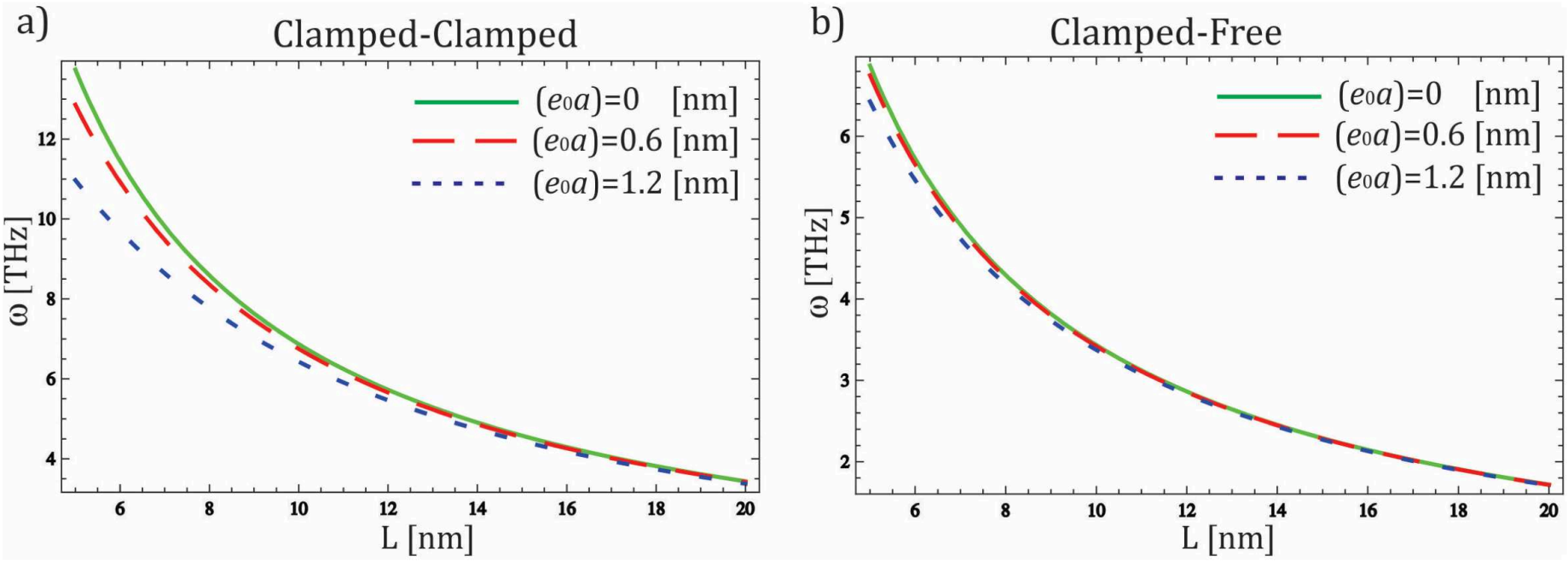
- Single-walled carbon nanotube (SWCNT) (5, 5): The following dimensions and values of parameters are used to obtain the results ρ =9517 [kg/m^3] E =6.85 [TPa] L =12.2 [mn] n =1
- The results are obtained for clamped-free boundary conditions and different values of ($e_0 a$) and compared with the results for the natural resonant frequency obtained by the molecular dynamics simulation in: 'Cao, G., Chen, X., Kysar, J. W. (2006). Thermal vibration and apparent thermal contraction of single-walled carbon nanotubes,Journal of the Mechanics and Physics of Solids, 54(6), 1206-1236.'

Nonlocal parameter					MD simulation
e_0a=0 nm	e_0a=0.5 nm	e_0a=1 nm	e_0a=1.5 nm	e_0a=2 nm	
0.549763	0.548627	0.545262	0.539788	0.532395	0.544

Comparison of the lower nonlocal natural frequency $f = \omega_1/2\pi$ of a nanorod model given in (THz) with the MD simulation for the armchair SWCNT (5, 5).

Numerical results

- Single-walled carbon nanotube (SWCNT) armchair (8, 8): The following dimensions and values of parameters are used to obtain the results ρ =2300 [kg/m^3] E =1.1 [TPa] h =0.34 [mn] n =1
- The results are obtained for both the boundary conditions and different values of the length L.

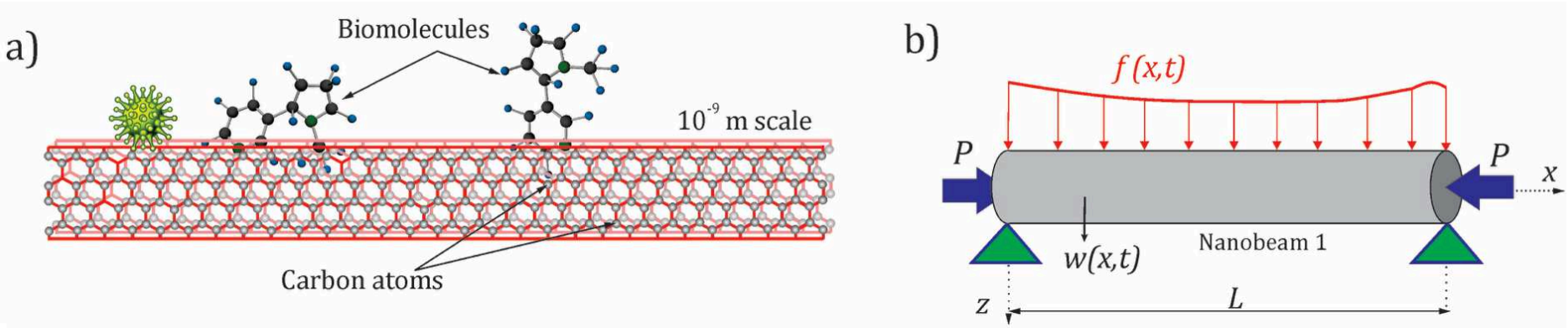


Fundamental natural frequencies for the longitudinal vibration of a nanorod; a) Clamped-Clamped BC, and b) Clamped-Free BC.

Nonlocal Euler-Bernoulli beam theory

- Euler-Bernoulli is the simplest beam theory for bending vibration
- We consider a beam with axial load P, external distributed applied load $q(x,t)$, density ρ, Young's modulus E, area A, moment of inertia I
- The equation of motion is given by

$$\rho A\frac{\partial^2 w}{\partial t^2} + P\frac{\partial^2 w}{\partial x^2} - q(x,t) + EI\frac{\partial^4 w}{\partial x^4} = (e_0 a)^2 \frac{\partial^2}{\partial x^2}\left(\rho A\frac{\partial^2 w}{\partial t^2} + P\frac{\partial^2 w}{\partial x^2} - q(x,t)\right) \quad (27)$$



Single-walled carbon nanotube (SWCNT) with externally attached biological particles: a) Physical model and b) Mechanical model.

Simply supported boundary conditions

- The boundary conditions for simply supported nonlocal Euler-Bernoulli?s nanobeam of the length L assumes that the deflections and bending moments at the ends of the nanobeam are equal to zero.
- At $x = 0$

$$w(0,t) = 0$$

$$M_f = \left[(e_0 a)^2 \frac{\partial^2}{\partial x^2}\left(\rho A \frac{\partial^2 w}{\partial t^2} + P\frac{\partial^2 w}{\partial x^2} - q(x,t)\right) - EI\frac{\partial^2 w}{\partial x^2}\right]_{x=0} = 0 \tag{28}$$

- At $x = L$

$$w(L,t) = 0$$

$$M_f = \left[(e_0 a)^2 \frac{\partial^2}{\partial x^2}\left(\rho A \frac{\partial^2 w}{\partial t^2} + P\frac{\partial^2 w}{\partial x^2} - q(x,t)\right) - EI\frac{\partial^2 w}{\partial x^2}\right]_{x=L} = 0 \tag{29}$$

Free vibration of nonlocal Euler-Bernoulli beams

- For the free vibration, ignoring transverse load q and the axial load P, we have the governing equation

$$\rho A\frac{\partial^2 w}{\partial t^2}+EI\frac{\partial^4 w}{\partial x^4}=(e_0 a)^2\frac{\partial^2}{\partial x^2}\left(\rho A\frac{\partial^2 w}{\partial t^2}\right) \tag{30}$$

- Supposing the harmonic motion of the nanobeam, we assume the solution for transverse displacements as

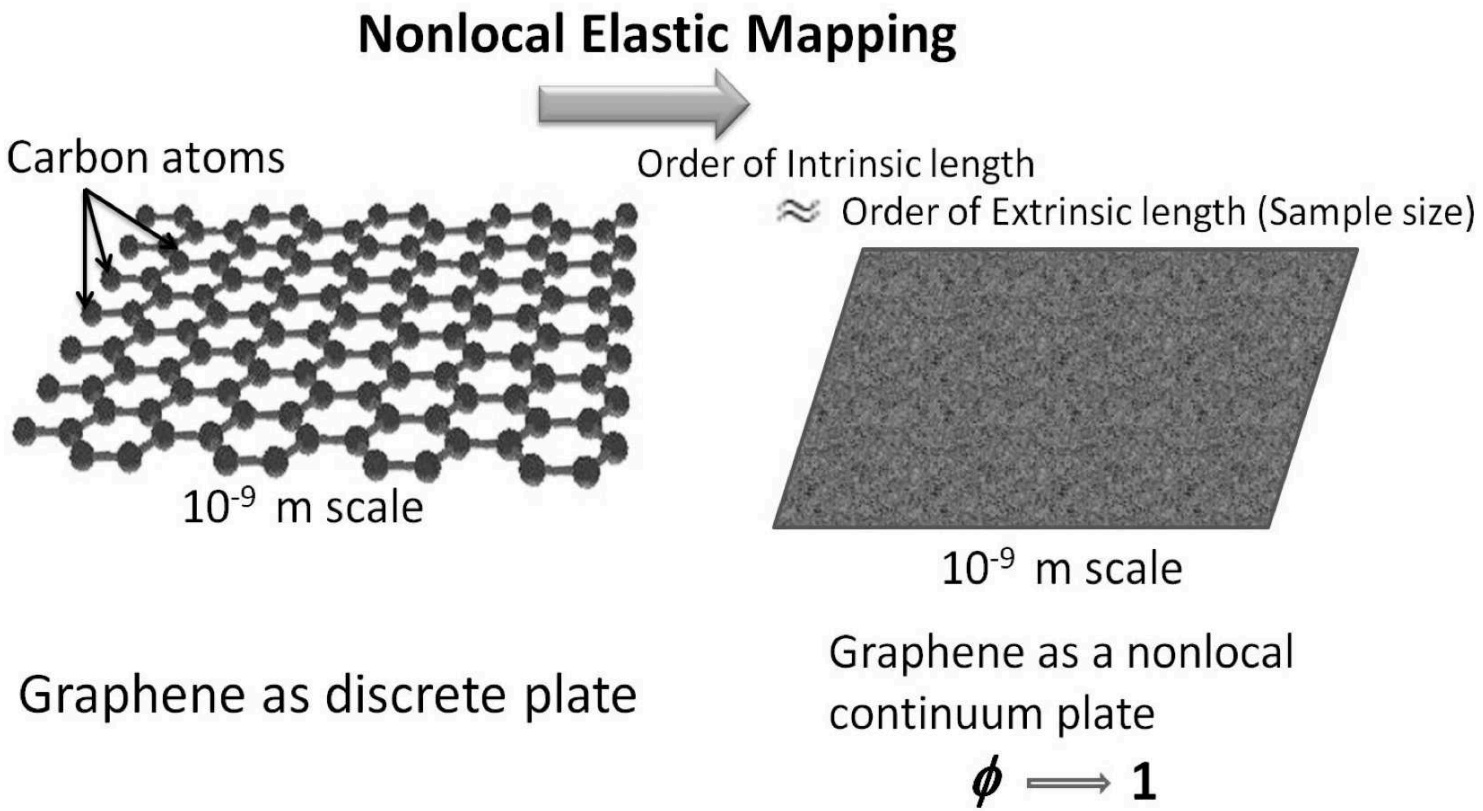
$$w(x,t)=\sum_{n=1}^{\infty} W_n \sin(\alpha_n x)e^{\mathrm{i}\omega_n t} \tag{31}$$

where $\mathrm{i}=\sqrt{-1}$, $\alpha_n = n\pi/L$, W_n are the amplitudes and ω_n is the natural frequency with n denoting the mode number.

- Substituting this in the equation of motion, the closed-from expression of the natural frequencies are given by

$$\omega_n=\sqrt{\frac{EI}{\rho A}}\frac{\alpha_n^2}{\sqrt{1+\alpha_n^2(e_0 a)^2}},\qquad n=1,2,3,\cdots \tag{32}$$

Nonlocal plate for graphene sheets



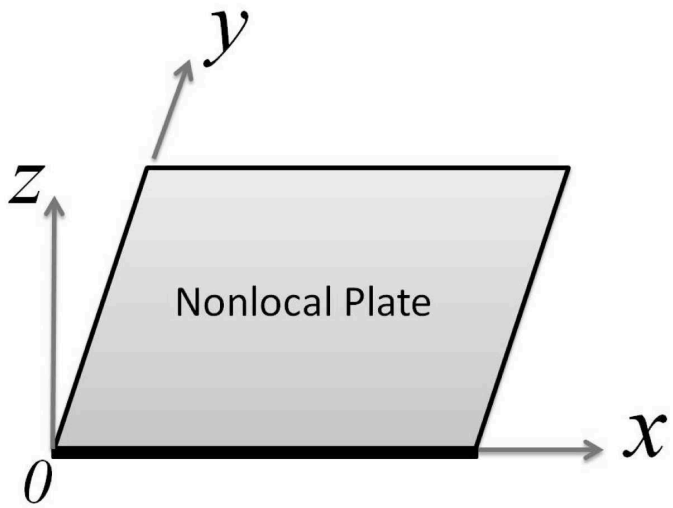
- The carbon atoms of graphene at small-scale is considered to be nonlocal in nature. Stress at a point not only depends on the strain at that point but on the strains of all the points in the body. By using this concept, the discrete graphene sheets can be modeled as continuum nonlocal elastic plate.

Equation of motion of nonlocal plate

- Equation of motion for free vibration

$$D\nabla^4 w(x,y,t) + \rho h\left(1-(e_0 a)^2\nabla^2\right)\left\{\frac{\partial^2 w(x,y,t)}{\partial t^2}\right\} = 0 \qquad (33)$$

- 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, ν is the Poisson's ratio, ρ is the density, $e_0 a$ is the nonlocal parameter and $w(x,y,t)$ is the transverse displacement.



Free vibration of simply-supported nonlocal plates

- The boundary conditions for a simply supported nano-plate ($L \times W$) are considered as $w(0,y) = w(L,y) = w(x,0) = w(x,W) = 0$ and nonlocal moment $M(0,y) = M(L,y) = M(x,0) = M(x,W) = 0$.
- For simply supported boundary conditions, the local and nonlocal boundary conditions are generally equivalent. However for other arbitrary boundary conditions local and nonlocal boundary condition would be different.
- We assume the solution as

$$w(x,y,t) = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} W_{mn}\sin(m\pi x/L)\sin(n\pi y/W)ye^{i\omega_{mn}t} \qquad (34)$$

  where ω_{mn} are the natural frequencies.
- Substituting this in Eq. (33), we can obtain the natural frequencies as

$$\omega_{mn} = \sqrt{\frac{D}{\rho h}}\frac{\psi_{mn}^2}{\sqrt{1+\psi_{mn}^2(e_0 a)^2}}, \quad \psi_{mn} = \sqrt{(m\pi/L)^2 + (m\pi/W)^2},$$

$$m, n = 1, 2, 3, \cdots \qquad (35)$$

Nonlocal finite element method

- Significant research efforts have taken place in the analysis of nano structures modelled as a continuum.
- While the results have given significant insights, the analysis is normally restricted to single-structure (e.g, a beam or a plate) with simple boundary conditions and no damping.
- In the future complex nanoscale structures will be used for next generation nano electro mechanical systems.
- Therefore, it is necessary to have the ability for design and analysis of damped built-up structures.
- The finite element approach for nanoscale structures can provide this generality.
- Work on nonlocal finite elements is in its infancy stage.

FEM for nonlocal dynamic systems

- 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.

Axial vibration of nanorods

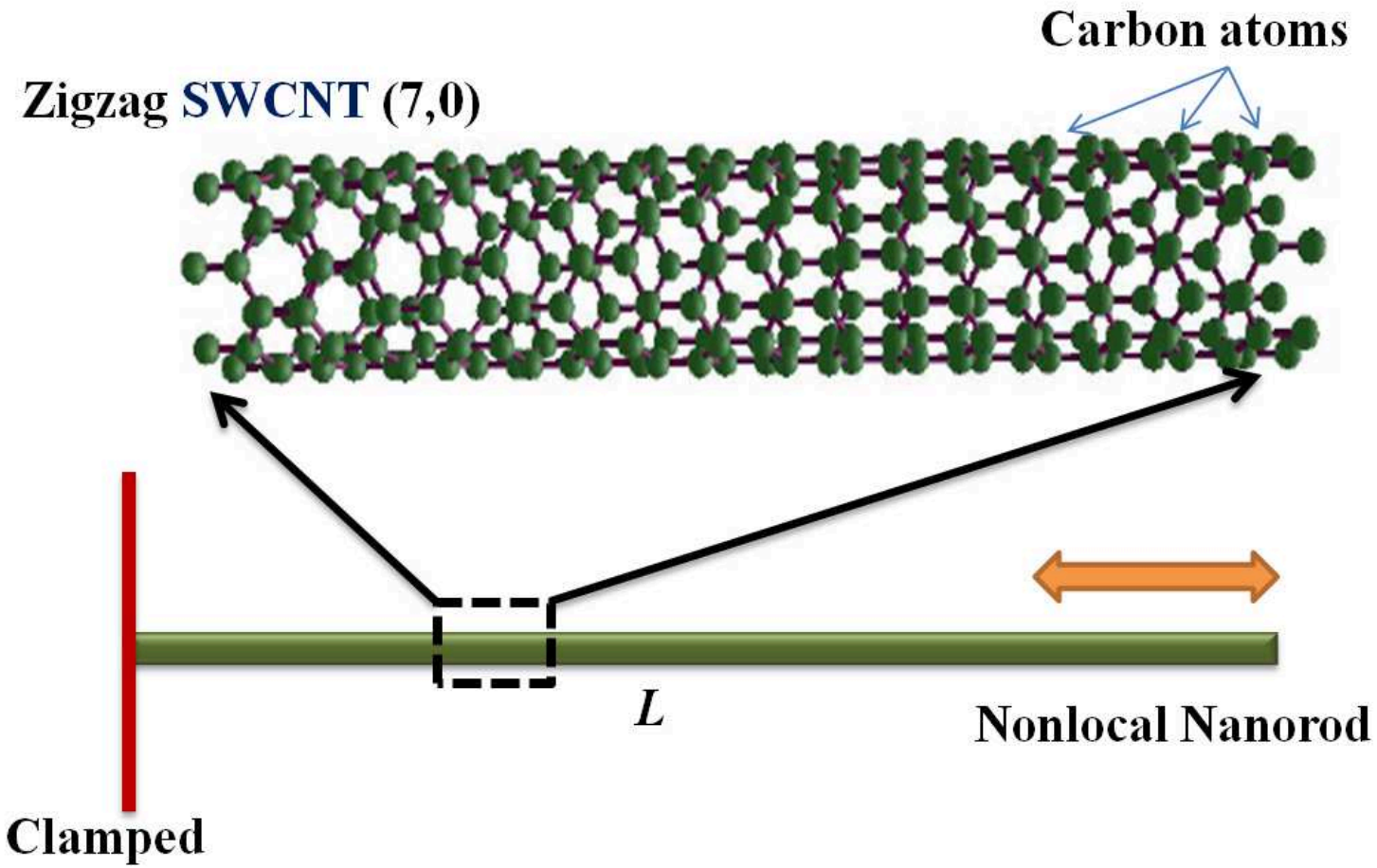


Figure: Axial vibration of a zigzag (7, 0) single-walled carbon nanotube (SWCNT) with clamped-free boundary condition.

Axial vibration of nanorods

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

$$EA\frac{\partial^2 U(x,t)}{\partial x^2} + \widehat{c}_1\frac{\partial^3 U(x,t)}{\partial x^2 \partial t} = \widehat{c}_2\frac{\partial U(x,t)}{\partial t} + \left(1 - (e_0 a)^2\frac{\partial^2}{\partial x^2}\right)\left\{m\frac{\partial^2 U(x,t)}{\partial t^2} + F(x,t)\right\} \quad (36)$$

- 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.

Nonlocal element matrices

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

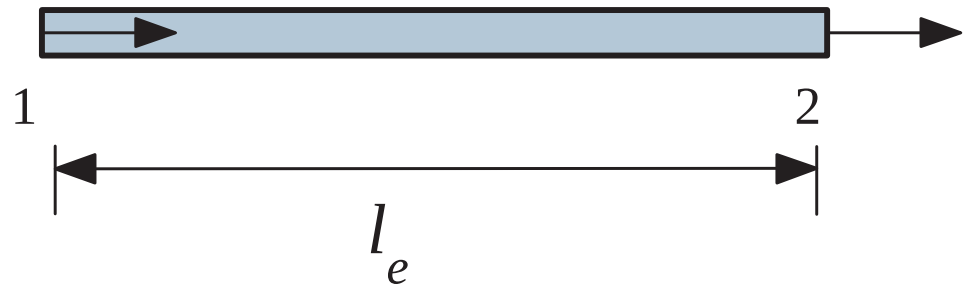


Figure: A nonlocal element for the axially vibrating rod with two nodes. It has two degrees of freedom and the displacement field within the element is expressed by linear shape functions.

- 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

$$\mathbf{N}(x) = [N_1(x), N_2(x)]^T = [1 - x/\ell_e, x/\ell_e]^T \tag{37}$$

Nonlocal element matrices

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

$$\mathbf{K}_e = EA\int_0^{\ell_e} \frac{d\mathbf{N}(x)}{dx}\frac{d\mathbf{N}^T(x)}{dx}\mathrm{d}x = \frac{EA}{\ell_e}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \tag{38}$$

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

$$\begin{aligned}\mathbf{M}_e &= m\int_0^{\ell_e} \mathbf{N}(x)\mathbf{N}^T(x)\mathrm{d}x + m(e_0a)^2\int_0^{\ell_e} \frac{d\mathbf{N}(x)}{dx}\frac{d\mathbf{N}^T(x)}{dx}\mathrm{d}x \\ &= \frac{m\ell_e}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} + \left(\frac{e_0a}{\ell_e}\right)^2 m\ell_e\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\end{aligned} \tag{39}$$

- For the special case when the rod is local, the mass matrix derived above reduces to the classical mass matrix[25, 26] as $e_0a = 0$. 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.

Bending vibration of nanobeams

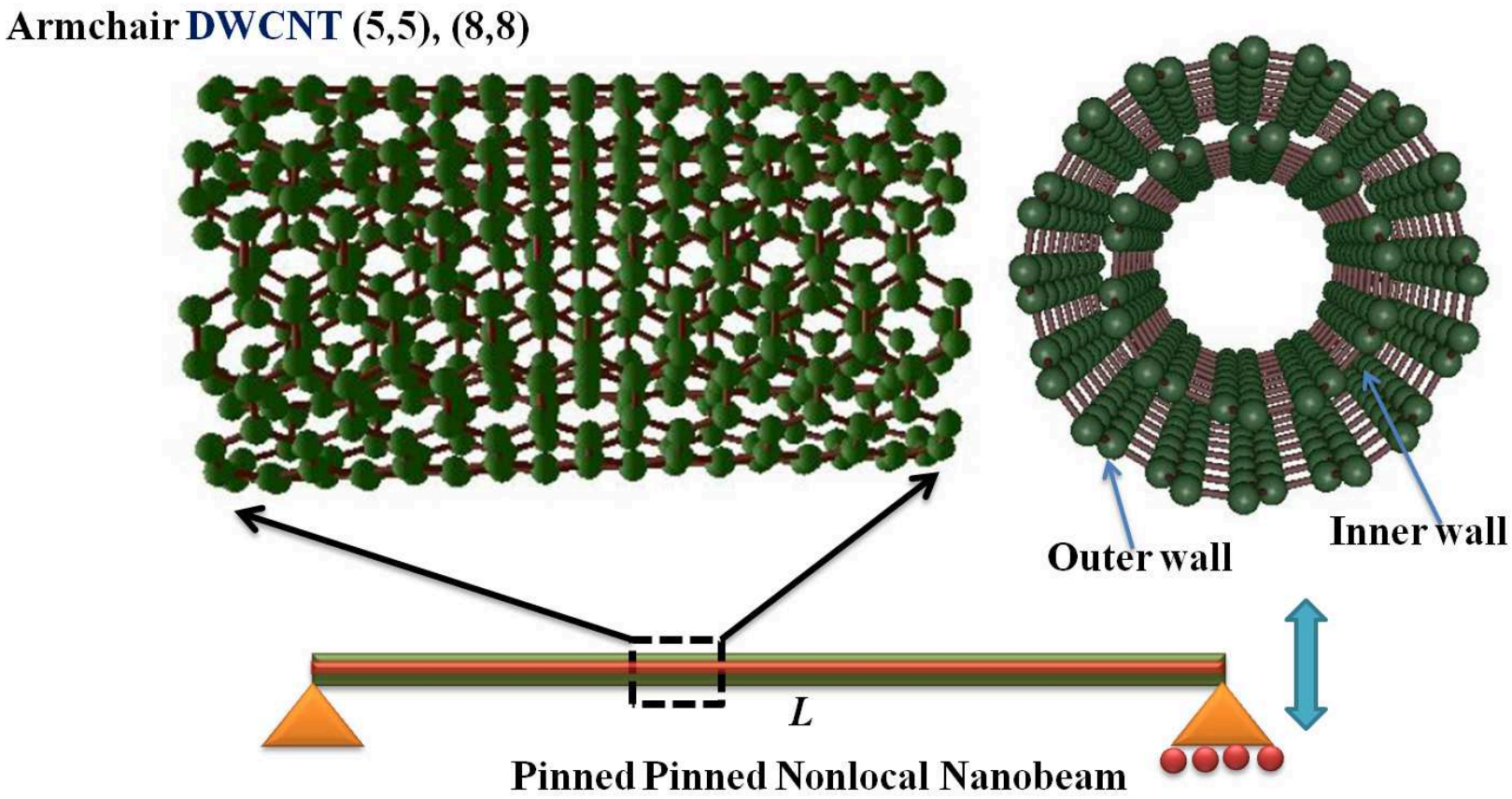


Figure: Bending vibration of an armchair (5, 5), (8, 8) double-walled carbon nanotube (DWCNT) with pinned-pinned boundary condition.

Bending vibration of nanobeams

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

$$EI\frac{\partial^4 V(x,t)}{\partial x^4} + m\left(1-(e_0 a)^2\frac{\partial^2}{\partial x^2}\right)\left\{\frac{\partial^2 V(x,t)}{\partial t^2}\right\} + \widehat{c}_1\frac{\partial^5 V(x,t)}{\partial x^4 \partial t} + \widehat{c}_2\frac{\partial V(x,t)}{\partial t} = \left(1-(e_0 a)^2\frac{\partial^2}{\partial x^2}\right)\{F(x,t)\} \quad (40)$$

- 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.

Nonlocal element matrices

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

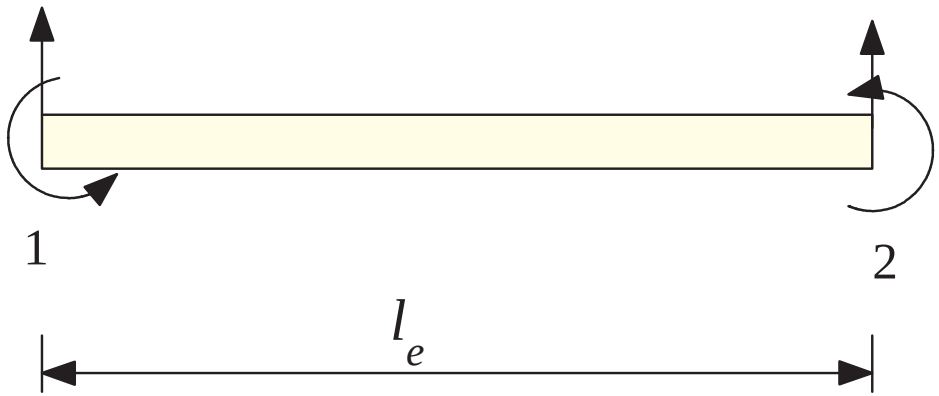


Figure: A nonlocal element for the bending vibration of a beam. It has two nodes and four degrees of freedom. The displacement field within the element is expressed by cubic shape functions.

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

Nonlocal element matrices

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

$$\mathbf{N}(x) = [N_1(x), N_2(x), N_3(x), N_4(x)]^T \tag{41}$$

where

$$\begin{aligned} N_1(x) &= 1 - 3\frac{x^2}{\ell_e^2} + 2\frac{x^3}{\ell_e^3}, & N_2(x) &= x - 2\frac{x^2}{\ell_e} + \frac{x^3}{\ell_e^2}, \\ N_3(x) &= 3\frac{x^2}{\ell_e^2} - 2\frac{x^3}{\ell_e^3}, & N_4(x) &= -\frac{x^2}{\ell_e} + \frac{x^3}{\ell_e^2} \end{aligned} \tag{42}$$

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

$$\mathbf{K}_e = EI \int_0^{\ell_e} \frac{d^2\mathbf{N}(x)}{dx^2} \frac{d^2\mathbf{N}^T(x)}{dx^2} \mathrm{d}x = \frac{EI}{\ell_e^3} \begin{bmatrix} 12 & 6\ell_e & -12 & 6\ell_e \\ 6\ell_e & 4\ell_e^2 & -6\ell_e & 2\ell_e^2 \\ -12 & -6\ell_e & 12 & -6\ell_e^2 \\ 6\ell_e & 2\ell_e^2 & -6\ell_e & 4\ell_e^2 \end{bmatrix} \tag{43}$$

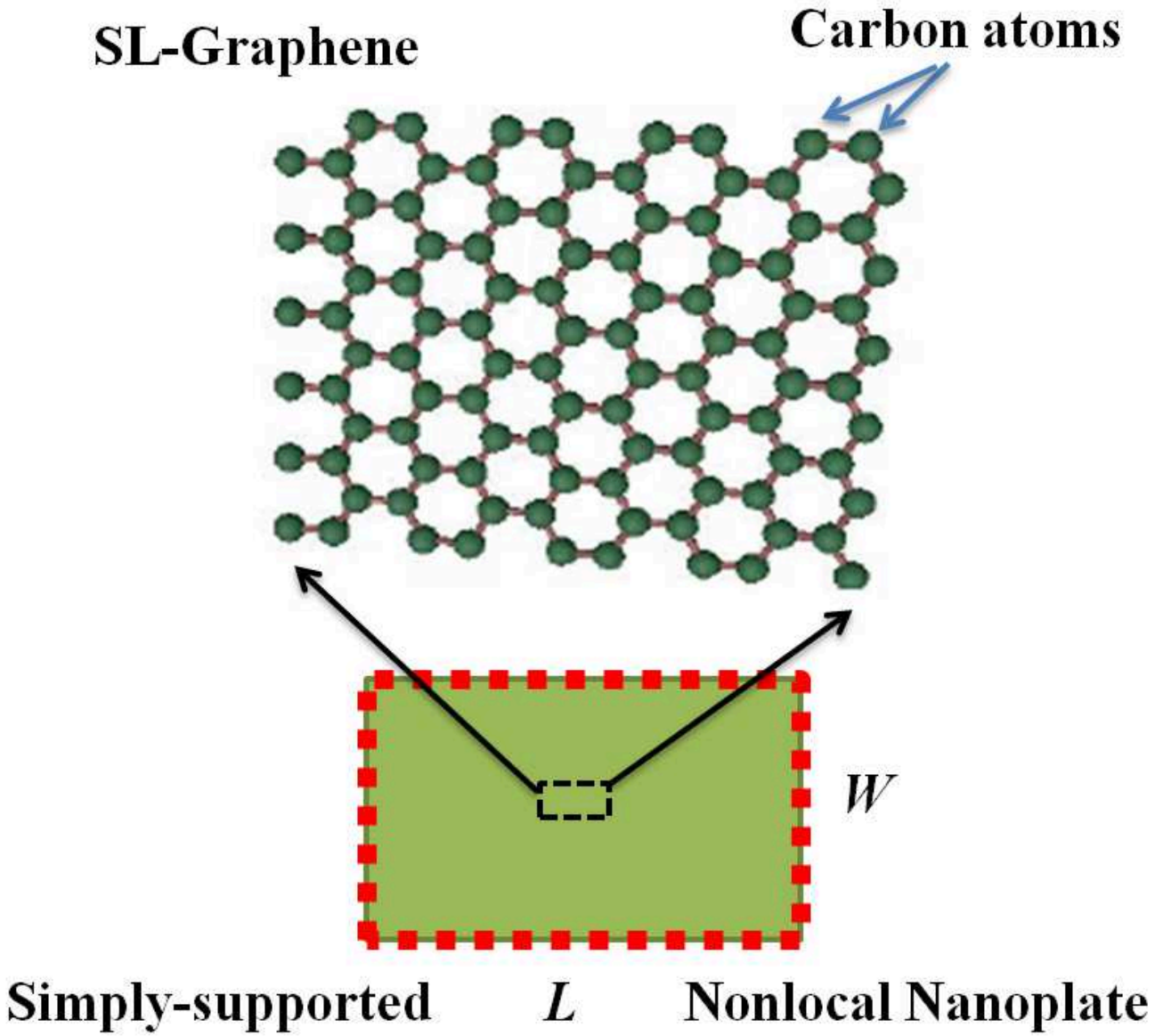
Nonlocal element matrices

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

$$\mathbf{M}_e = m\int_0^{\ell_e}\mathbf{N}(x)\mathbf{N}^T(x)\mathrm{d}x + m(e_0a)^2\int_0^{\ell_e}\frac{d\mathbf{N}(x)}{dx}\frac{d\mathbf{N}^T(x)}{dx}\mathrm{d}x$$
$$= \frac{m\ell_e}{420}\begin{bmatrix} 156 & 22\ell_e & 54 & -13\ell_e \\ 22\ell_e & 4\ell_e^2 & 13\ell_e & -3\ell_e^2 \\ 54 & 13\ell_e & 156 & -22\ell_e \\ -13\ell_e & -3\ell_e^2 & -22\ell_e & 4\ell_e^2 \end{bmatrix} \tag{44}$$
$$+\left(\frac{e_0a}{\ell_e}\right)^2\frac{m\ell_e}{30}\begin{bmatrix} 36 & 3\ell_e & -36 & 3\ell_e \\ 3\ell_e & 4\ell_e^2 & -3\ell_e & -\ell_e^2 \\ -36 & -3\ell_e & 36 & -3\ell_e \\ 3\ell_e & -\ell_e^2 & -3\ell_e & 4\ell_e^2 \end{bmatrix}$$

- For the special case when the beam is local, the mass matrix derived above reduces to the classical mass matrix [25, 26] as $e_0a = 0$.

Transverse vibration of nanoplates



Transverse vibration of nanoplates

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

$$D\nabla^4 V(x,y,t) + m\left(1-(e_0 a)^2\nabla^2\right)\left\{\frac{\partial^2 V(x,y,t)}{\partial t^2}\right\} + \widehat{c}_1\nabla^4\frac{\partial V(x,y,t)}{\partial t} + \widehat{c}_2\frac{\partial V(x,y,t)}{\partial t} = \left(1-(e_0 a)^2\nabla^2\right)\{F(x,y,t)\} \quad (45)$$

- 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, ν 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.

Nonlocal element matrices

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

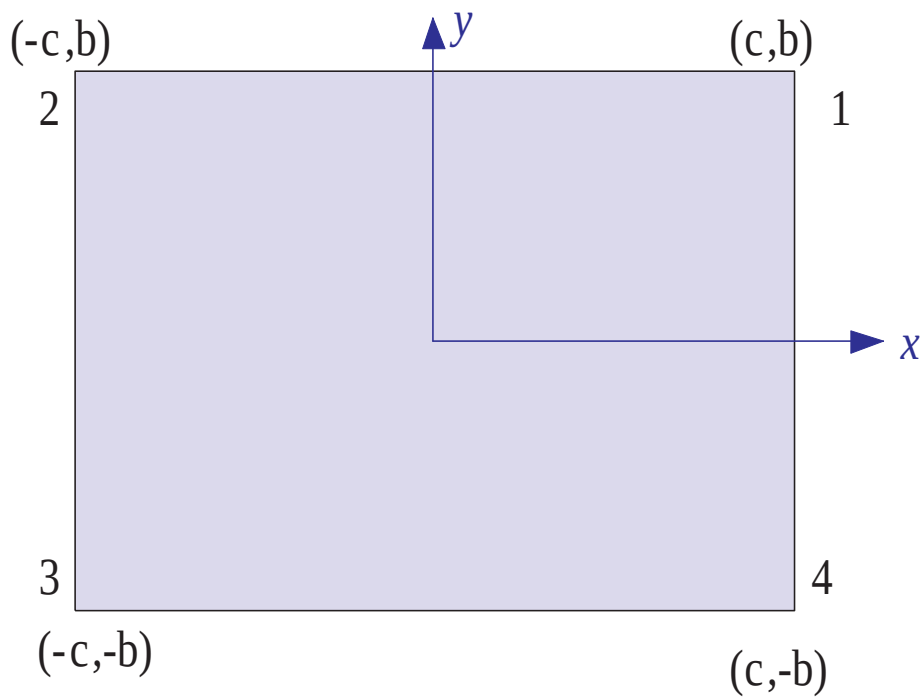


Figure: A nonlocal element for the bending vibration of a plate. It has four nodes and twelve degrees of freedom. The displacement field within the element is expressed by cubic shape functions in both directions.

Nonlocal element matrices

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

$$\mathbf{N}(x, y) = \mathbf{C}_e^{-1} \alpha(x, y) \tag{46}$$

- Here the vector of polynomials is given by

$$\alpha(x, y) = \begin{bmatrix} 1 & x & y & x^2 & xy & y^2 & x^3 & x^2y & xy^2 & y^3 & x^3y & xy^3 \end{bmatrix}^T \tag{47}$$

- The 12×12 coefficient matrix can be obtained in closed-form.

Nonlocal element matrices

- Using the shape functions in Eq. (46), the stiffness matrix can be obtained using the conventional variational formulation [26] as

$$\mathbf{K}_e = \int_{A_e} \mathbf{B}^T \mathbf{E} \mathbf{B} \mathrm{d}A_e \tag{48}$$

- In the preceding equation $\mathbf{B}$ is the strain-displacement matrix, and the matrix $\mathbf{E}$ is given by

$$\mathbf{E} = D \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{bmatrix} \tag{49}$$

- Evaluating the integral in Eq. (48), we can obtain the element stiffness matrix in closed-form as

$$\mathbf{K}_e = \frac{Eh^3}{12(1-\nu^2)} \mathbf{C}^{-1\,T} \mathbf{k}_e \mathbf{C}^{-1} \tag{50}$$

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

Nonlocal element matrices

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

$$\begin{aligned}\mathbf{M}_e = \rho h \int_{A_e} \Big\{ & \mathbf{N}(x,y)\mathbf{N}^T(x,y) \\ & + (e_0 a)^2 \left(\frac{\partial \mathbf{N}(x,y)}{\partial x} \frac{d\mathbf{N}^T(x,y)}{dx} + \frac{\partial \mathbf{N}(x,y)}{\partial x} \frac{d\mathbf{N}^T(x,y)}{dx} \right) \Big\} \, \mathrm{d}A_e \qquad (51) \\ & = \mathbf{M}_{0_e} + \left(\frac{e_0 a}{c} \right)^2 \mathbf{M}_{x_e} + \left(\frac{e_0 a}{b} \right)^2 \mathbf{M}_{y_e}\end{aligned}$$

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

Nonlocal element matrices

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

$$\begin{bmatrix}
276 & 66b & 42c & -276 & -66b & 42c & -102 & 39b & 21c & 102 & -39b & 21c \\
66b & 24b^2 & 0 & -66b & -24b^2 & 0 & -39b & 18b^2 & 0 & 39b & -18b^2 & 0 \\
42c & 0 & 112c^2 & -42c & 0 & -28c^2 & -21c & 0 & -14c^2 & 21c & 0 & 56c^2 \\
-276 & -66b & -42c & 276 & 66b & -42c & 102 & -39b & -21c & -102 & 39b & -21c \\
-66b & -24b^2 & 0 & 66b & 24b^2 & 0 & 39b & -18b^2 & 0 & -39b & 18b^2 & 0 \\
42c & 0 & -28c^2 & -42c & 0 & 112c^2 & -21c & 0 & 56c^2 & 21c & 0 & -14c^2 \\
-102 & -39b & -21c & 102 & 39b & -21c & 276 & -66b & -42c & -276 & 66b & -42c \\
39b & 18b^2 & 0 & -39b & -18b^2 & 0 & -66b & 24b^2 & 0 & 66b & -24b^2 & 0 \\
21c & 0 & -14c^2 & -21c & 0 & 56c^2 & -42c & 0 & 112c^2 & 42c & 0 & -28c^2 \\
102 & 39b & 21c & -102 & -39b & 21c & -276 & 66b & 42c & 276 & -66b & 42c \\
-39b & -18b^2 & 0 & 39b & 18b^2 & 0 & 66b & -24b^2 & 0 & -66b & 24b^2 & 0 \\
21c & 0 & 56c^2 & -21c & 0 & -14c^2 & -42c & 0 & -28c^2 & 42c & 0 & 112c^2
\end{bmatrix} \tag{52}$$

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

$$\begin{bmatrix}
276 & 42b & 66c & 102 & 21b & -39c & -102 & 21b & 39c & -276 & 42b & -66c \\
42b & 112b^2 & 0 & 21b & 56b^2 & 0 & -21b & -14b^2 & 0 & -42b & -28b^2 & 0 \\
66c & 0 & 24c^2 & 39c & 0 & -18c^2 & -39c & 0 & 18c^2 & -66c & 0 & -24c^2 \\
102 & 21b & 39c & 276 & 42b & -66c & -276 & 42b & 66c & -102 & 21b & -39c \\
21b & 56b^2 & 0 & 42b & 112b^2 & 0 & -42b & -28b^2 & 0 & -21b & -14b^2 & 0 \\
-39c & 0 & -18c^2 & -66c & 0 & 24c^2 & 66c & 0 & -24c^2 & 39c & 0 & 18c^2 \\
-102 & -21b & -39c & -276 & -42b & 66c & 276 & -42b & -66c & 102 & -21b & 39c \\
21b & -14b^2 & 0 & 42b & -28b^2 & 0 & -42b & 112b^2 & 0 & -21b & 56b^2 & 0 \\
39c & 0 & 18c^2 & 66c & 0 & -24c^2 & -66c & 0 & 24c^2 & -39c & 0 & -18c^2 \\
-276 & -42b & -66c & -102 & -21b & 39c & 102 & -21b & -39c & 276 & -42b & 66c \\
42b & -28b^2 & 0 & 21b & -14b^2 & 0 & -21b & 56b^2 & 0 & -42b & 112b^2 & 0 \\
-66c & 0 & -24c^2 & -39c & 0 & 18c^2 & 39c & 0 & -18c^2 & 66c & 0 & 24c^2
\end{bmatrix} \tag{53}$$

Nonlocal element matrices: Summary

- 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

$$\mathbf{M}_e = \mathbf{M}_{0_e} + \mathbf{M}_{\mu_e} \tag{54}$$

  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.

Global system matrices

- 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

$$\mathbf{M} = \mathbf{M}_0 + \mathbf{M}_\mu \tag{55}$$

- 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:

$$\mathbf{M}_\mu = \left(\frac{e_0 a}{L}\right)^2 \widehat{\mathbf{M}}_\mu \tag{56}$$

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 $e_0 a$.

Nonlocal modal analysis

- 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.

Conditions for classical normal modes

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

$$[\mathbf{M}_0 + \mathbf{M}_\mu]\,\ddot{\mathbf{u}}(t) + \mathbf{C}\dot{\mathbf{u}}(t) + \mathbf{K}\mathbf{u}(t) = \mathbf{f}(t) \tag{57}$$

- 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

$$\mathbf{M}_0\ddot{\mathbf{u}}_0(t) + \mathbf{C}\dot{\mathbf{u}}_0(t) + \mathbf{K}\mathbf{u}_0(t) = \mathbf{f}(t) \tag{58}$$

  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

$$\mathbf{K}\mathbf{x}_j = \omega_j^2\mathbf{M}_0\mathbf{x}_j, \quad \forall\, j = 1, 2, \ldots, n \tag{59}$$

Dynamics of the local system

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

$$\mathbf{x}_k^T \mathbf{M}_0 \mathbf{x}_j = \delta_{kj} \tag{60}$$

$$\text{and} \quad \mathbf{x}_k^T \mathbf{K} \mathbf{x}_j = \omega_j^2 \delta_{kj}, \quad \forall\, k, j = 1, 2, \ldots, n \tag{61}$$

  where δ_{kj} is the Kroneker delta function. We construct the local modal matrix

$$\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n] \in \mathbb{R}^n \tag{62}$$

- The local modal matrix can be used to diagonalize the local system (58) 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

$$\mathbf{C}\mathbf{M}_0^{-1}\mathbf{K} = \mathbf{K}\mathbf{M}_0^{-1}\mathbf{C} \tag{63}$$

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

Conditions for classical normal modes

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

$$\left(\mathbf{I}_n + \mathbf{M}_0^{-1}\mathbf{M}_\mu\right)\ddot{\mathbf{u}}(t) + \left(\mathbf{M}_0^{-1}\mathbf{K}\right)\mathbf{u}(t) = \mathbf{M}_0^{-1}\mathbf{f}(t) \tag{64}$$

- 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

$$\left(\mathbf{M}_0^{-1}\mathbf{K}\right)\left(\mathbf{M}_0^{-1}\mathbf{M}_\mu\right) = \left(\mathbf{M}_0^{-1}\mathbf{M}_\mu\right)\left(\mathbf{M}_0^{-1}\mathbf{K}\right) \tag{65}$$

$$\text{or} \quad \mathbf{K}\mathbf{M}_0^{-1}\mathbf{M}_\mu = \mathbf{M}_\mu\mathbf{M}_0^{-1}\mathbf{K} \tag{66}$$

- 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

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

$$\mathbf{K}\mathbf{u}_j = \lambda_j^2 \left[\mathbf{M}_0 + \mathbf{M}_\mu\right] \mathbf{u}_j, \quad \forall\, j = 1, 2, \ldots, n \tag{67}$$

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

$$\mathbf{U} = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_n] \in \mathbb{R}^n \tag{68}$$

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.

Nonlocal normal modes: Damped systems

- Under certain restrictive condition it may be possible to diagonalise the damped nonlocal system using classical normal modes.
- Premultiplying the equation of motion (57) 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. (63) and (66), we also need a third condition

$$\mathbf{C}\mathbf{M}_0^{-1}\mathbf{M}_\mu = \mathbf{M}_\mu\mathbf{M}_0^{-1}\mathbf{C} \tag{69}$$

- If we consider the diagonalization of the nonlocal system by the nonlocal modal matrix in (68), 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. (63) 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.

Approximate nonlocal 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 (57), 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 (ω_I^2), local eigenvectors $\mathbf{x}_I$, $\forall\, I = 1, \ldots, n$, form a complete set of vectors. For this reason each nonlocal normal mode $\mathbf{u}_j$ can be expanded as a linear combination of $\mathbf{x}_I$:

$$\mathbf{u}_j = \sum_{I=1}^{n} \alpha_I^{(j)} \mathbf{x}_I \tag{70}$$

- Without any loss of generality, we can assume that $\alpha_j^{(j)} = 1$ (normalization) which leaves us to determine $\alpha_I^{(j)}, \forall I \neq j$.
- Substituting the expansion of $\mathbf{u}_j$ into the eigenvalue equation (67), one obtains

$$\left[-\lambda_j^2 \left(\mathbf{M}_0 + \mathbf{M}_\mu\right) + \mathbf{K}\right] \sum_{I=1}^{n} \alpha_I^{(j)} \mathbf{x}_I = \mathbf{0} \tag{71}$$

For the case when $\alpha_I^{(j)}$ are approximate, the error involving the projection in Eq. (70) can be expressed as

$$\boldsymbol{\varepsilon}_j = \sum_{I=1}^{n} \left[-\lambda_j^2 \left(\mathbf{M}_0 + \mathbf{M}_\mu\right) + \mathbf{K}\right] \alpha_I^{(j)} \mathbf{x}_I \tag{72}$$

Nonlocal natural frequencies

- 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

$$\varepsilon_j \perp \mathbf{x}_l \quad \text{or} \quad \mathbf{x}_k^T \varepsilon_j = 0 \quad \forall\ k = 1, 2, \ldots, n \tag{73}$$

- Using the orthogonality property of the undamped local modes

$$\sum_{l=1}^{n} \left[-\lambda_j^2 \left(\delta_{kl} + M'_{\mu_{kl}} \right) + \omega_k^2 \delta_{kl} \right] \alpha_l^{(j)} = 0 \tag{74}$$

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

$$\lambda_j \approx \frac{\omega_j}{\sqrt{1 + M'_{\mu_{jj}}}} \tag{75}$$

Nonlocal mode shapes

- When $k \neq j$, from Eq. (74) we have

$$\left[-\lambda_j^2\left(1+M'_{\mu_{kk}}\right)+\omega_k^2\right]\alpha_k^{(j)}-\lambda_j^2\sum_{l\neq k}^{n}\left(M'_{\mu_{kl}}\right)\alpha_l^{(j)}=0 \tag{76}$$

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

$$\left[-\lambda_j^2\left(1+M'_{\mu_{kk}}\right)+\omega_k^2\right]\alpha_k^{(j)}=\lambda_j^2\left[M'_{\mu_{kj}}+\sum_{l\neq k\neq j}^{n}M'_{\mu_{kl}}\alpha_l^{(j)}\right] \tag{77}$$

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

$$\mathbf{u}_j\approx\mathbf{x}_j+\sum_{k\neq j}^{n}\frac{\lambda_j^2}{\left(\lambda_k^2-\lambda_j^2\right)}\frac{M'_{\mu_{kj}}}{\left(1+M'_{\mu_{kk}}\right)}\mathbf{x}_k \tag{78}$$

Nonlocal normal modes

Equations (75) and (78) 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.

Frequency response of nonlocal systems

- Taking the Fourier transformation of the equation of motion (57) we have

$$\mathbf{D}(\mathrm{i}\omega)\bar{\mathbf{u}}(\mathrm{i}\omega) = \bar{\mathbf{f}}(\mathrm{i}\omega) \tag{79}$$

where the nonlocal dynamic stiffness matrix is given by

$$\mathbf{D}(\mathrm{i}\omega) = -\omega^2\left[\mathbf{M}_0 + \mathbf{M}_\mu\right] + \mathrm{i}\omega\mathbf{C} + \mathbf{K} \tag{80}$$

- In Eq. (79) $\bar{\mathbf{u}}(\mathrm{i}\omega)$ and $\bar{\mathbf{f}}(\mathrm{i}\omega)$ are respectively the Fourier transformations of the response and the forcing vectors.
- Using the local modal matrix (62), the dynamic stiffness matrix can be transformed to the modal coordinate as

$$\mathbf{D}'(\mathrm{i}\omega) = \mathbf{X}^T\mathbf{D}(\mathrm{i}\omega)\mathbf{X} = -\omega^2\left[\mathbf{I} + \mathbf{M}'_\mu\right] + \mathrm{i}\omega\mathbf{C}' + \mathbf{\Omega}^2 \tag{81}$$

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.

Frequency response of nonlocal systems

- We separate the diagonal and off-diagonal terms as

$$\mathbf{D}'(\mathrm{i}\omega) = \underbrace{-\omega^2\left[\mathbf{I}+\overline{\mathbf{M}}'_\mu\right]+\mathrm{i}\omega\overline{\mathbf{C}}'+\boldsymbol{\Omega}^2}_{\text{diagonal}} + \underbrace{\left(-\omega^2\Delta\mathbf{M}'_\mu+\mathrm{i}\omega\Delta\mathbf{C}'\right)}_{\text{off-diagonal}} \tag{82}$$

$$= \overline{\mathbf{D}}'(\mathrm{i}\omega)+\Delta\mathbf{D}'(\mathrm{i}\omega) \tag{83}$$

- The dynamic response of the system can be obtained as

$$\bar{\mathbf{u}}(\mathrm{i}\omega) = \mathbf{H}(\mathrm{i}\omega)\bar{\mathbf{f}}(\mathrm{i}\omega) = \left[\mathbf{X}\mathbf{D}'^{-1}(\mathrm{i}\omega)\mathbf{X}^T\right]\bar{\mathbf{f}}(\mathrm{i}\omega) \tag{84}$$

  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

$$\mathbf{D}'^{-1}(\mathrm{i}\omega) = \left[\overline{\mathbf{D}}'(\mathrm{i}\omega)\left(\mathbf{I}+\overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega)\Delta\mathbf{D}'(\mathrm{i}\omega)\right)\right]^{-1} \tag{85}$$

$$\approx \overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega)-\overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega)\Delta\mathbf{D}'(\mathrm{i}\omega)\overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega) \tag{86}$$

Frequency response of nonlocal systems

- Substituting the approximate expression of $\mathbf{D}'^{-1}(\mathrm{i}\omega)$ from Eq. (86) into the expression of the transfer function matrix in Eq. (84) we have

$$\mathbf{H}(\mathrm{i}\omega) = \left[\mathbf{X}\mathbf{D}'^{-1}(\mathrm{i}\omega)\mathbf{X}^T\right] \approx \overline{\mathbf{H}}'(\mathrm{i}\omega) - \Delta\mathbf{H}'(\mathrm{i}\omega) \tag{87}$$

where

$$\overline{\mathbf{H}}'(\mathrm{i}\omega) = \mathbf{X}\overline{\mathbf{D}}'(\mathrm{i}\omega)\mathbf{X}^T = \sum_{k=1}^{n} \frac{\mathbf{x}_k\mathbf{x}_k^T}{-\omega^2\left(1+M'_{\mu_{kk}}\right) + 2\mathrm{i}\omega\omega_k\zeta_k + \omega_k^2} \tag{88}$$

and $$\Delta\mathbf{H}'(\mathrm{i}\omega) = \mathbf{X}\overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega)\Delta\mathbf{D}'(\mathrm{i}\omega)\overline{\mathbf{D}}'^{-1}(\mathrm{i}\omega)\mathbf{X}^T \tag{89}$$

- Equation (87) 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 6.

Nonlocal transfer function

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 $\Delta\mathbf{M}'_\mu$ and the off-diagonal part of the of the modal damping matrix $\Delta\mathbf{C}'$. 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 $\Delta\mathbf{C}' = \mathbf{O}$. For this case error in the transfer function only depends on $\Delta\mathbf{M}'_\mu$.
- In general, error in the transfer function is expected to be higher for higher frequencies as both $\Delta\mathbf{C}'$ and $\Delta\mathbf{M}'_\mu$ are weighted by frequency ω.

The expressions of the nonlocal natural frequencies (75), nonlocal normal modes (78) and the nonlocal transfer function matrix (87) allow us to understand the dynamic characteristic of a nonlocal system in a qualitative and quantitative manner in the light of equivalent local systems.

Axial vibration of a single-walled carbon nanotube

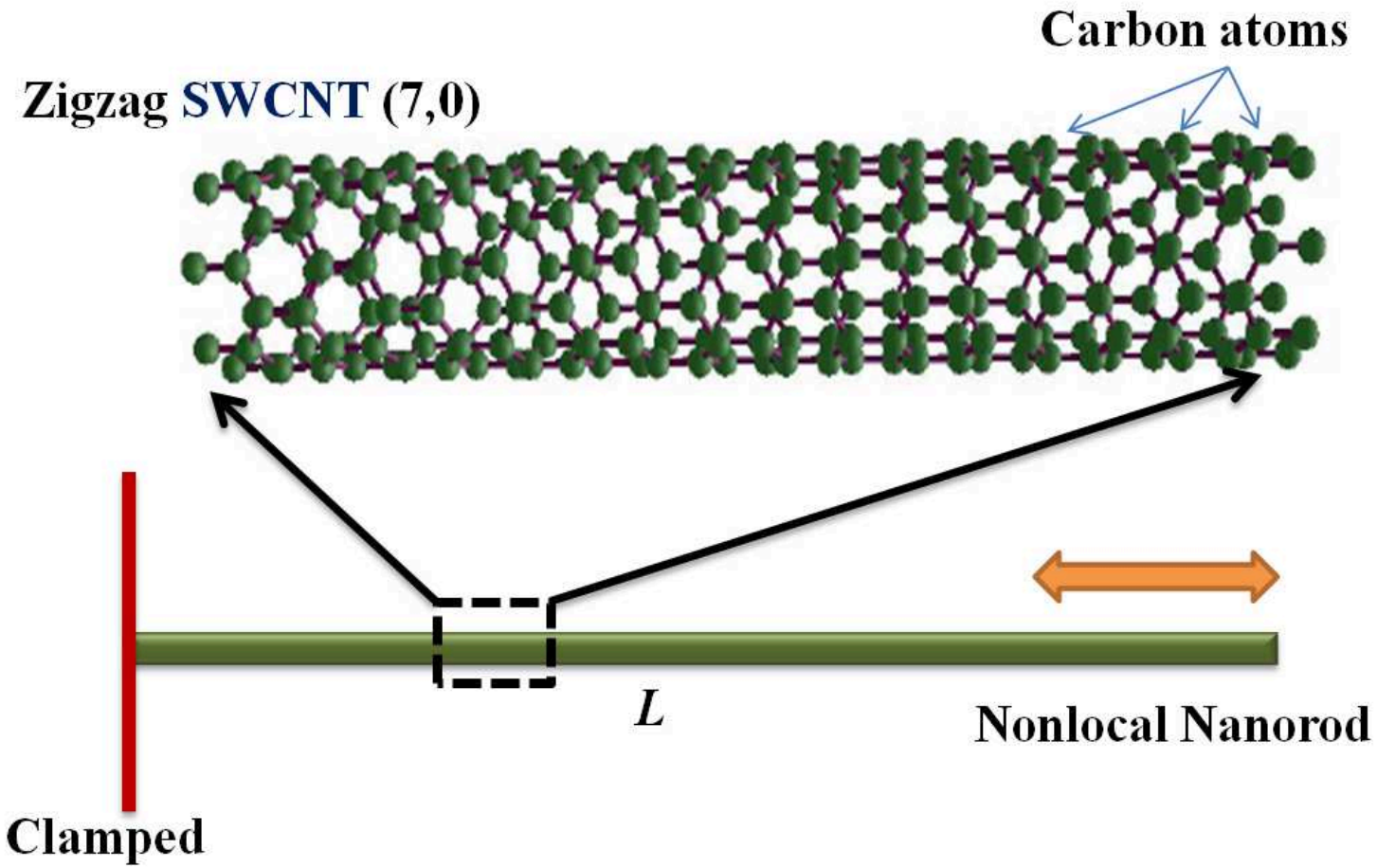


Figure: Axial vibration of a zigzag (7, 0) single-walled carbon nanotube (SWCNT) with clamped-free boundary condition.

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

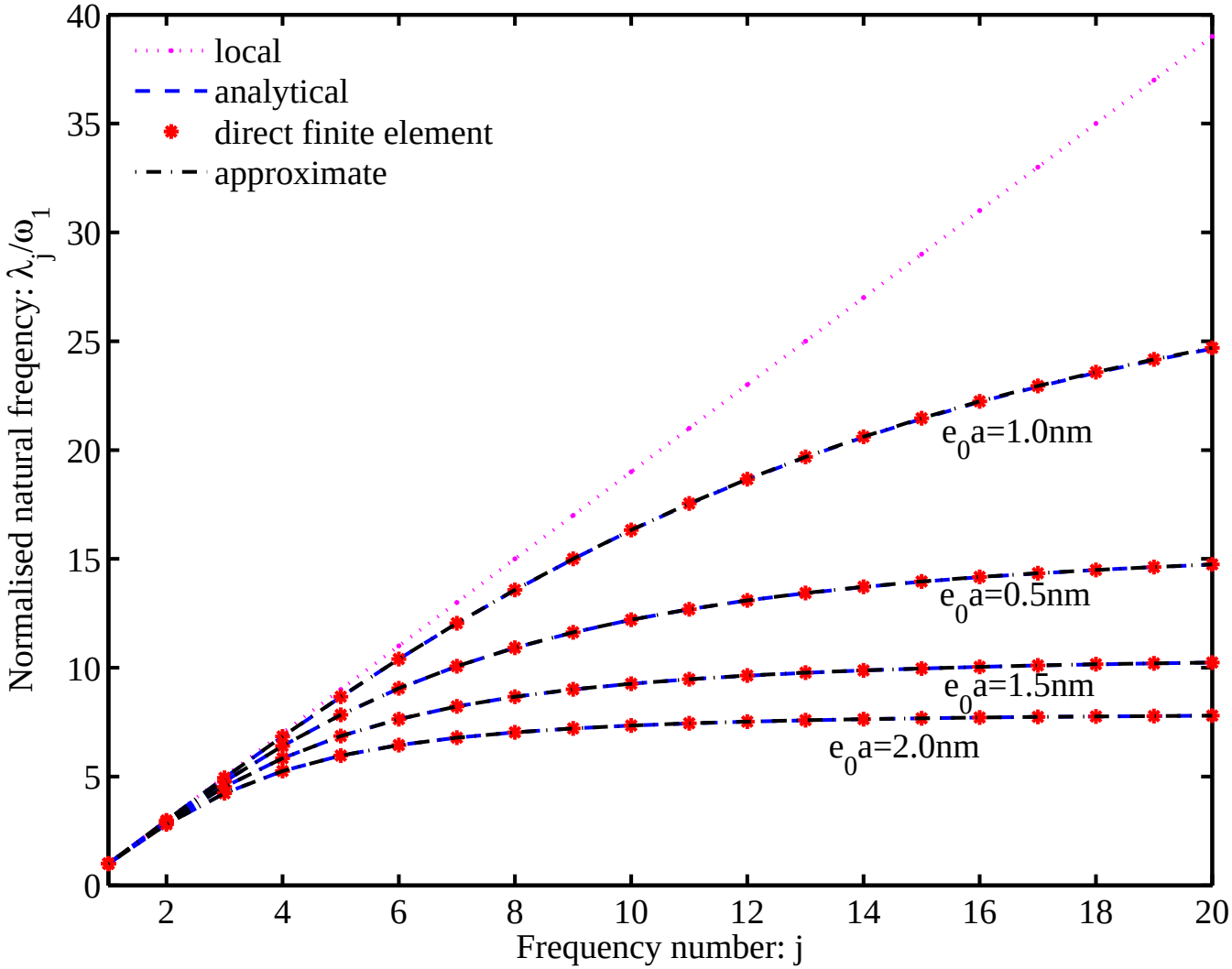
$$d_i = \frac{r}{\pi}\sqrt{n_i^2 + m_i^2 + n_i m_i} \tag{90}$$

  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

$$\lambda_j = \sqrt{\frac{EA}{m}}\frac{\sigma_j}{\sqrt{1+\sigma_j^2(e_0 a)^2}}, \quad \text{where} \quad \sigma_j = \frac{(2j-1)\pi}{2L}, \quad j = 1, 2, \cdots \tag{91}$$

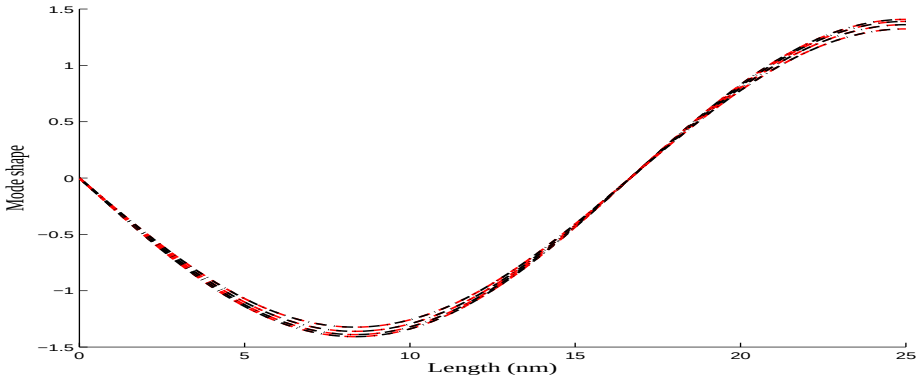
  EA is the axial rigidity and m is the mass per unit length of the SWCNT.
- For the finite element analysis the SWCNT is divided into 200 elements. The dimension of each of the system matrices become 200×200, that is $n = 200$.

Nonlocal axial natural frequencies of SWCNT

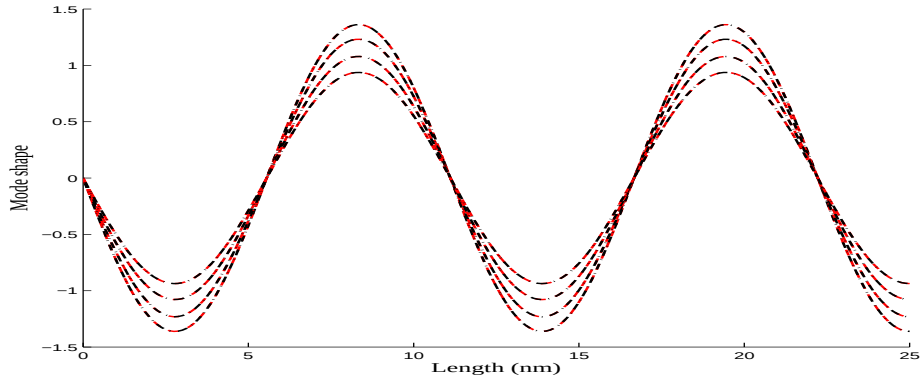


First 20 undamped natural frequencies for the axial vibration of SWCNT.

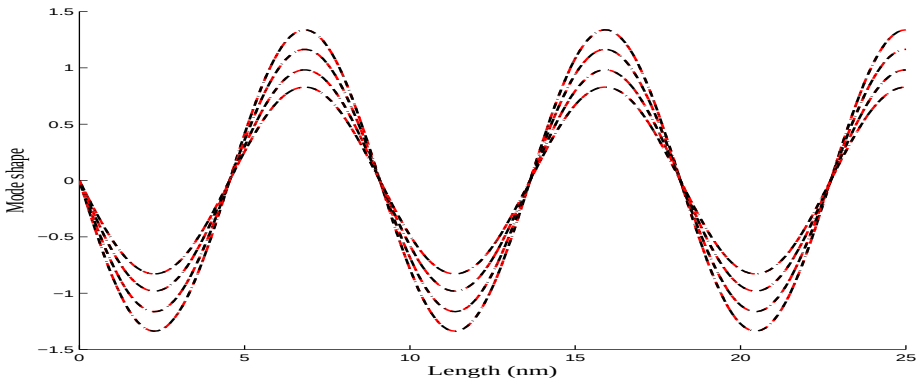
Nonlocal axial mode shapes of SWCNT



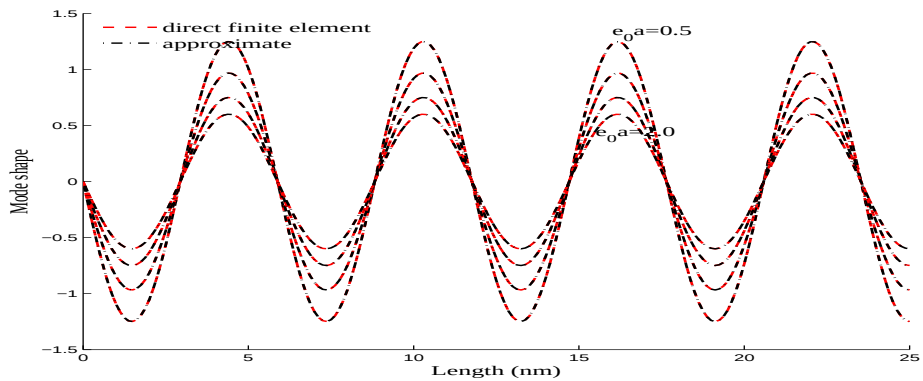
(a) Mode 2



(b) Mode 5



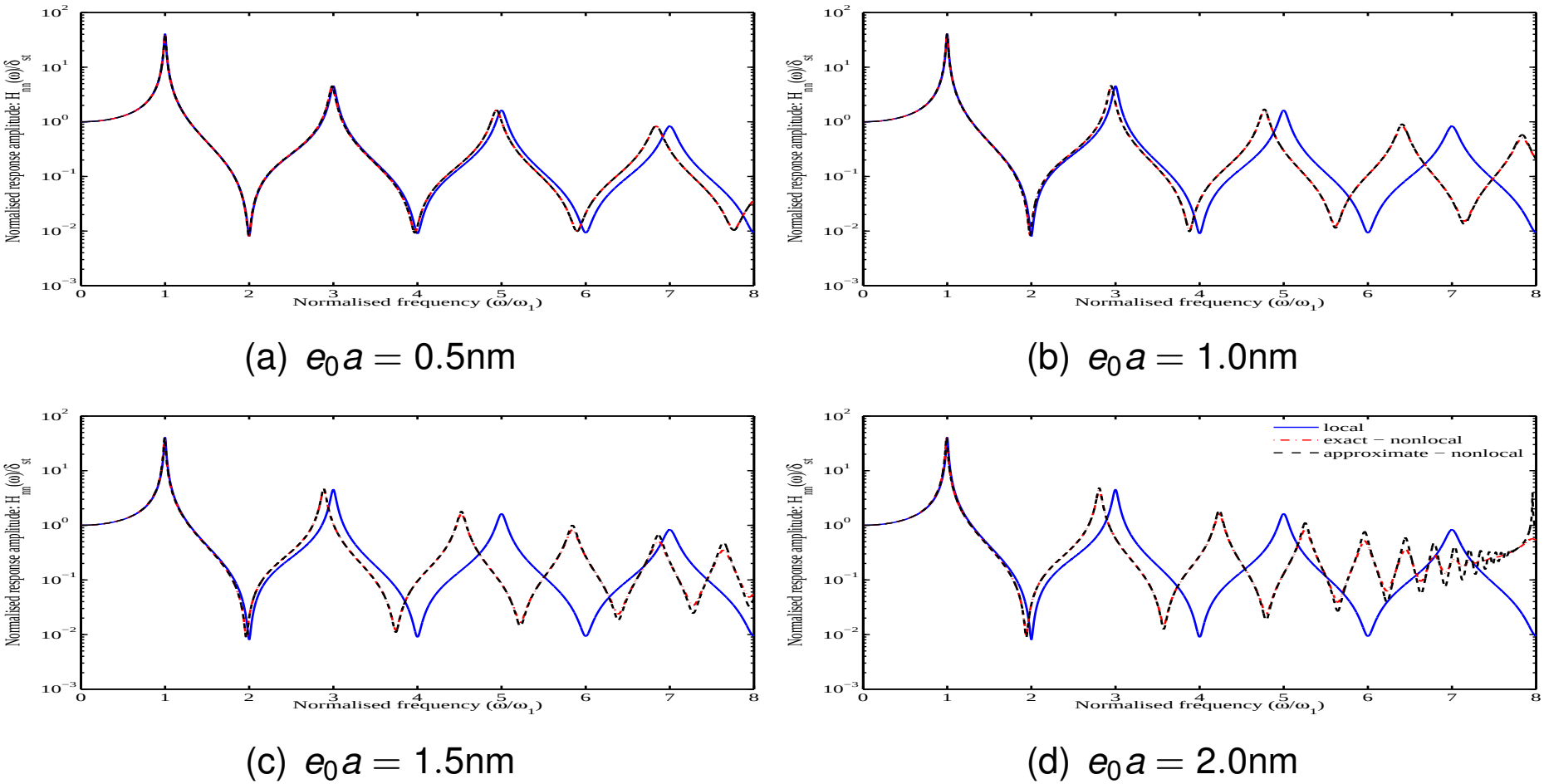
(c) Mode 6



(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 $e_0 a$, namely 0.5, 1.0, 1.5 and 2.0nm have been used.

Nonlocal frequency response of SWCNT



(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.

Bending vibration of a double-walled carbon nanotube

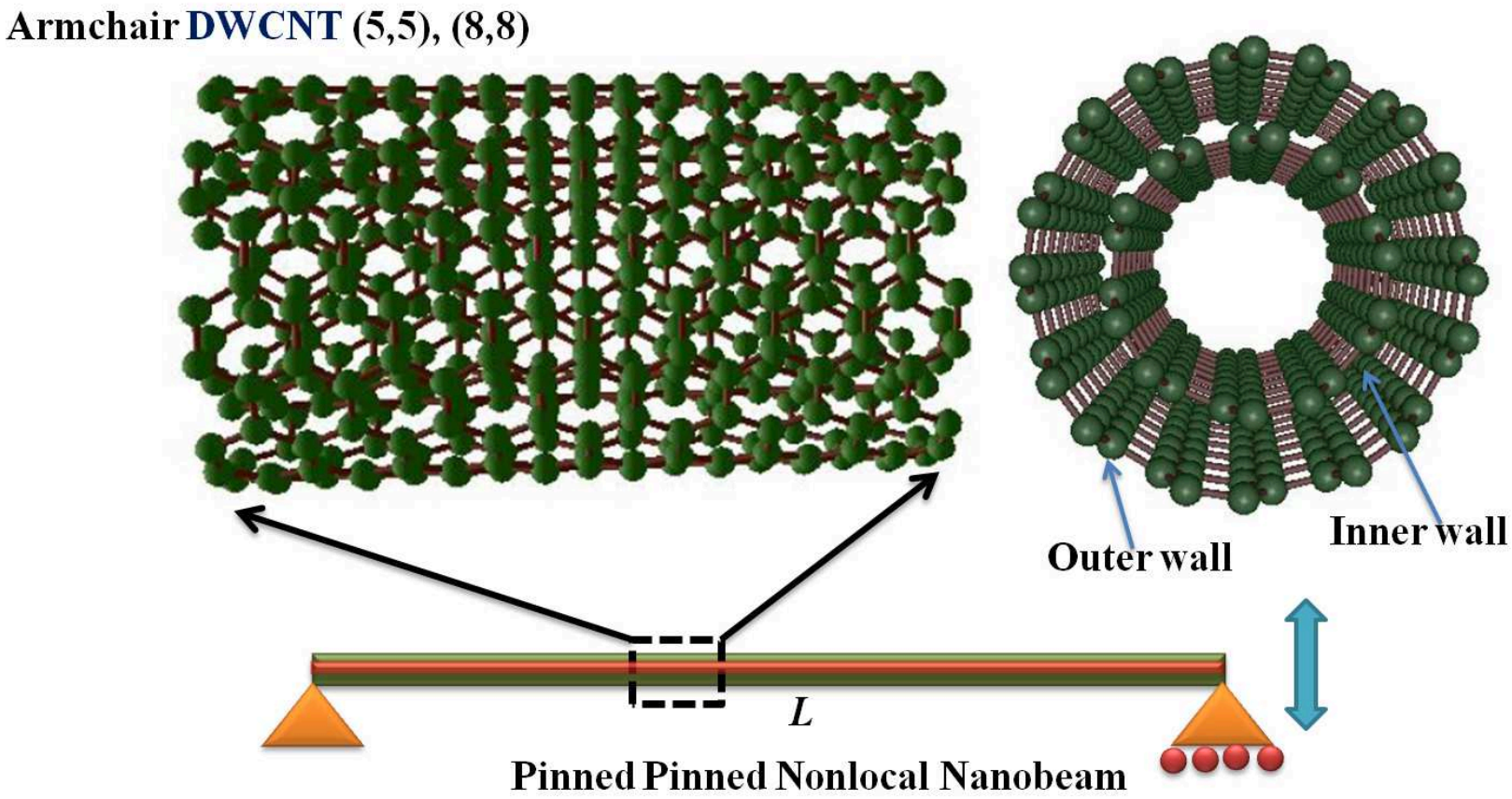


Figure: Bending vibration of an armchair (5, 5), (8, 8) double-walled carbon nanotube (DWCNT) with pinned-pinned boundary condition.

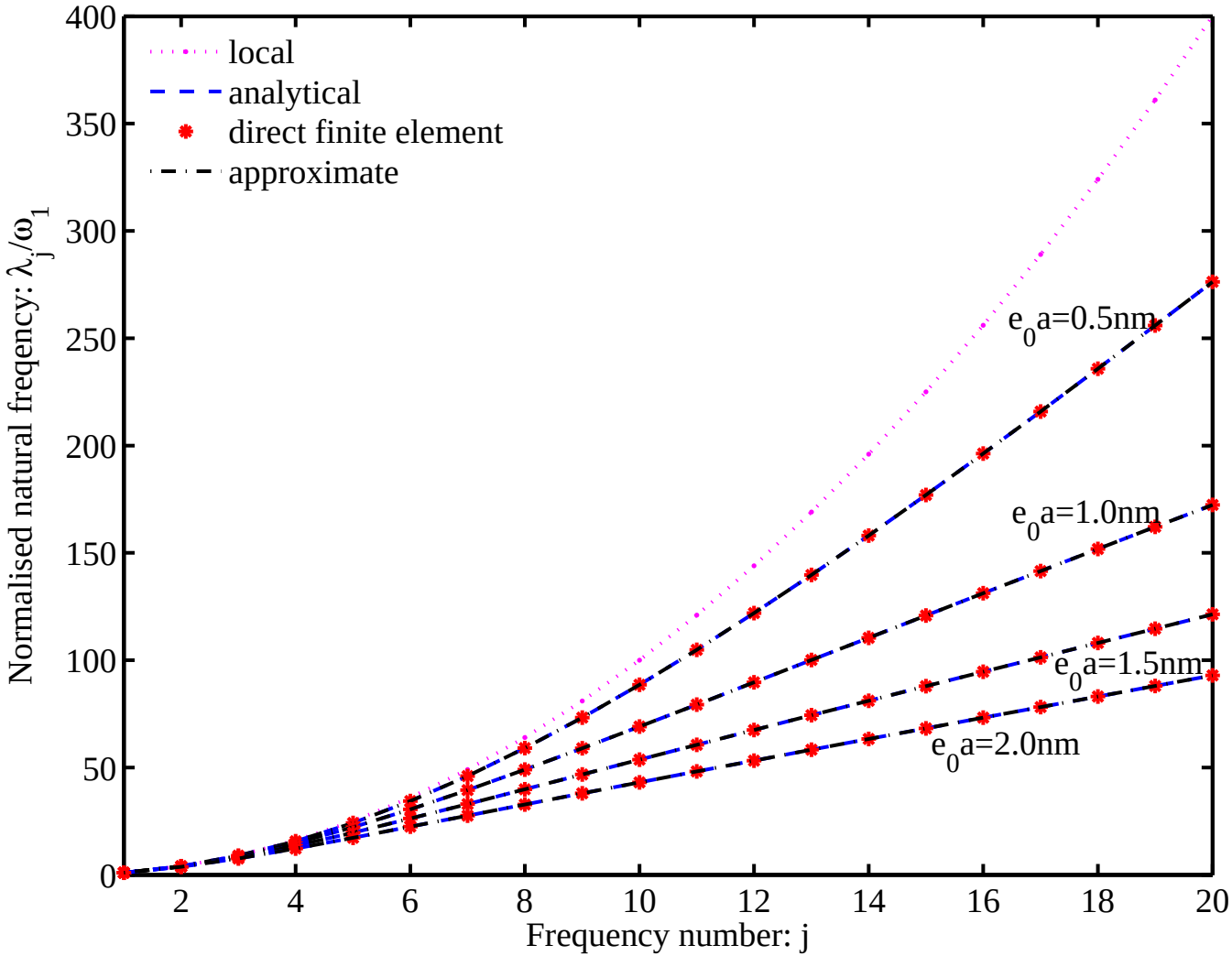
Bending vibration of a double-walled carbon nanotube

- 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.
- A constant modal damping factor of 1% for all the modes is assumed.
- We consider pinned-pinned boundary condition for the DWCNT. Undamped nonlocal natural frequencies can be obtained [11] as

$$\lambda_j = \sqrt{\frac{EI}{m}} \frac{\beta_j^2}{\sqrt{1 + \beta_j^2 (e_0 a)^2}} \quad \text{where} \quad \beta_j = j\pi/L, \quad j = 1, 2, \cdots \tag{92}$$

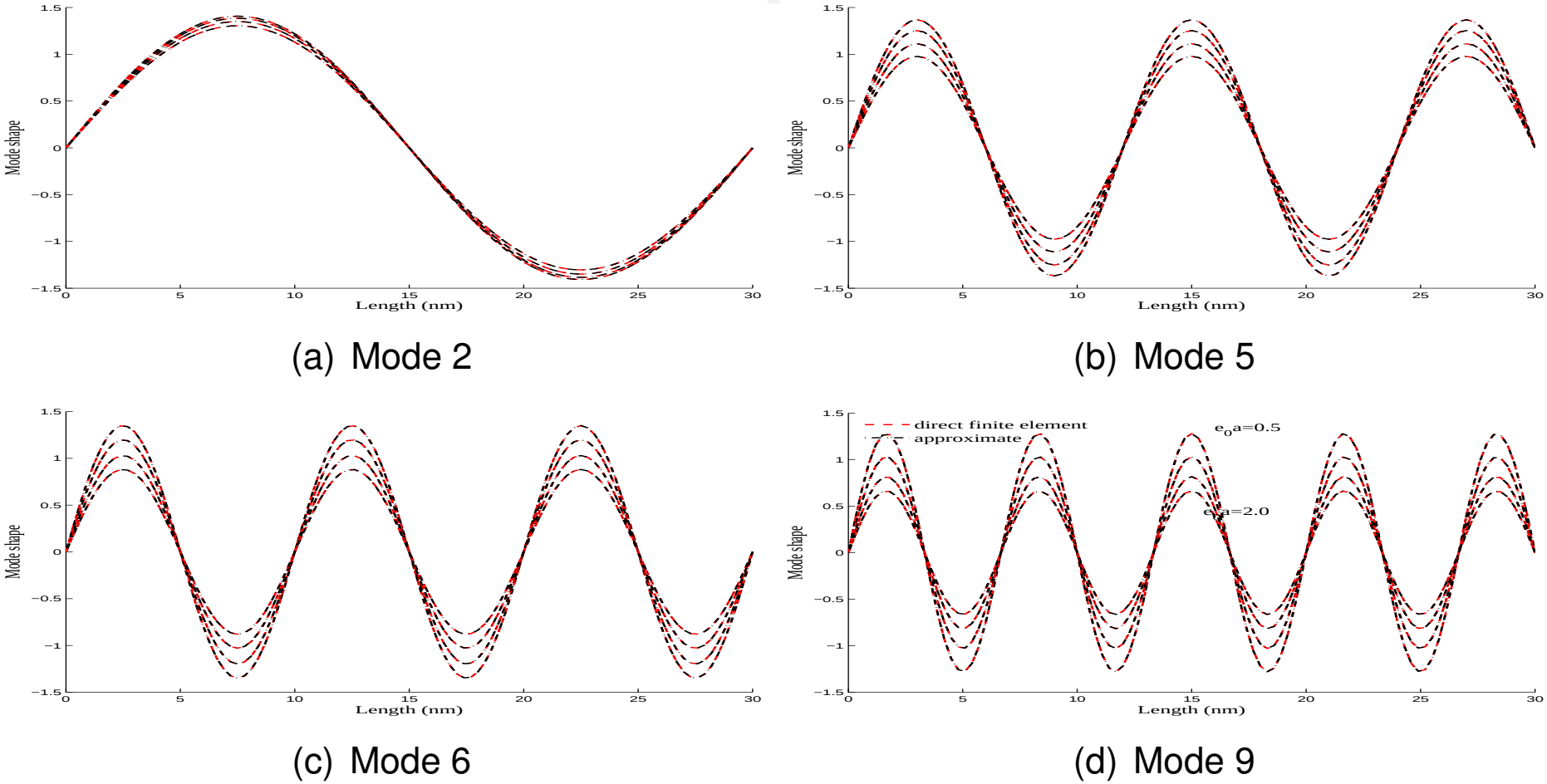
- For the finite element analysis the DWCNT is divided into 100 elements. The dimension of each of the system matrices become 200×200, that is $n = 200$.

Nonlocal bending natural frequencies of DWCNT



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

Nonlocal bending mode shapes of DWCNT



(a) Mode 2

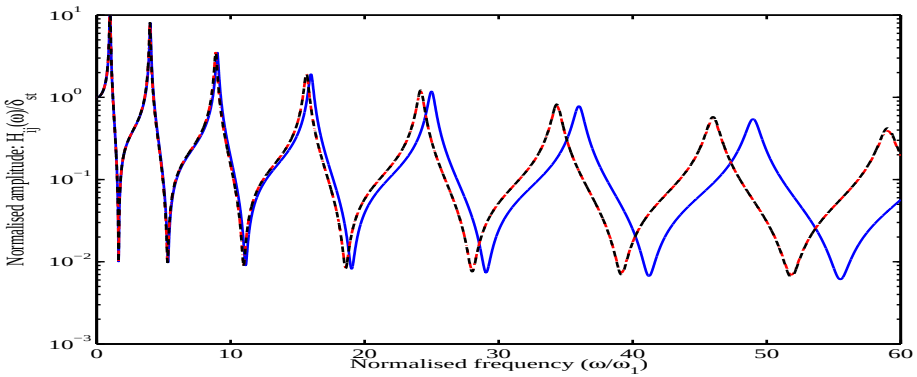
(b) Mode 5

(c) Mode 6

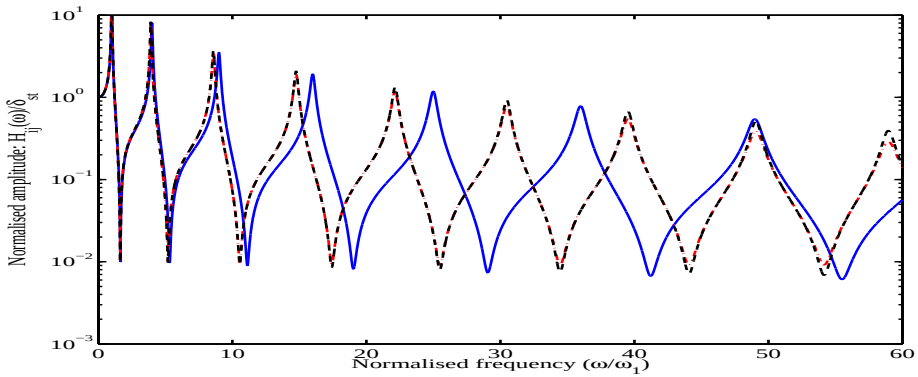
(d) Mode 9

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

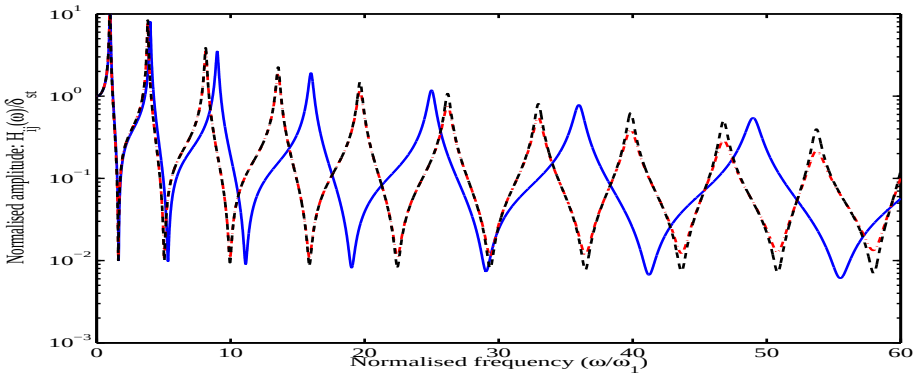
Nonlocal frequency response of DWCNT



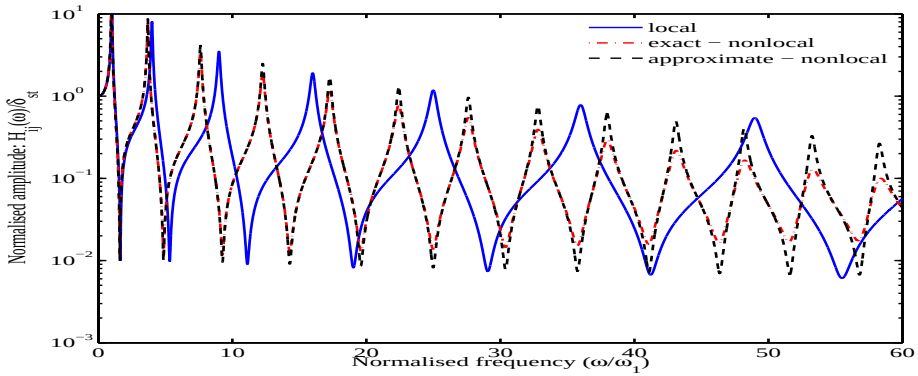
(a) $e_0 a = 0.5$nm



(b) $e_0 a = 1.0$nm



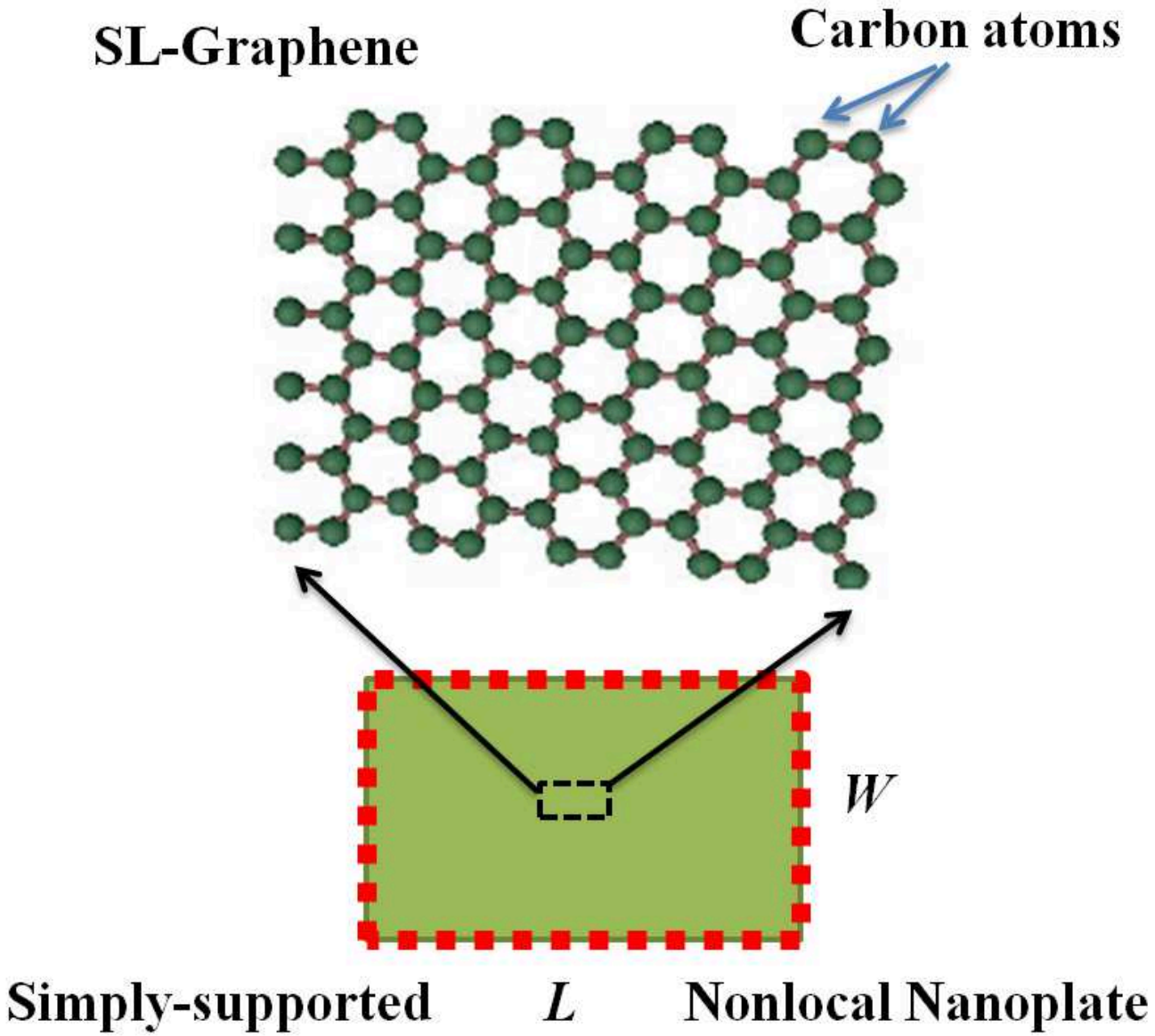
(c) $e_0 a = 1.5$nm



(d) $e_0 a = 2.0$nm

Figure: Amplitude of the normalised frequency response of the DWCNT $H_{ij}(\omega)$ for $i = 6, j = 8$ 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



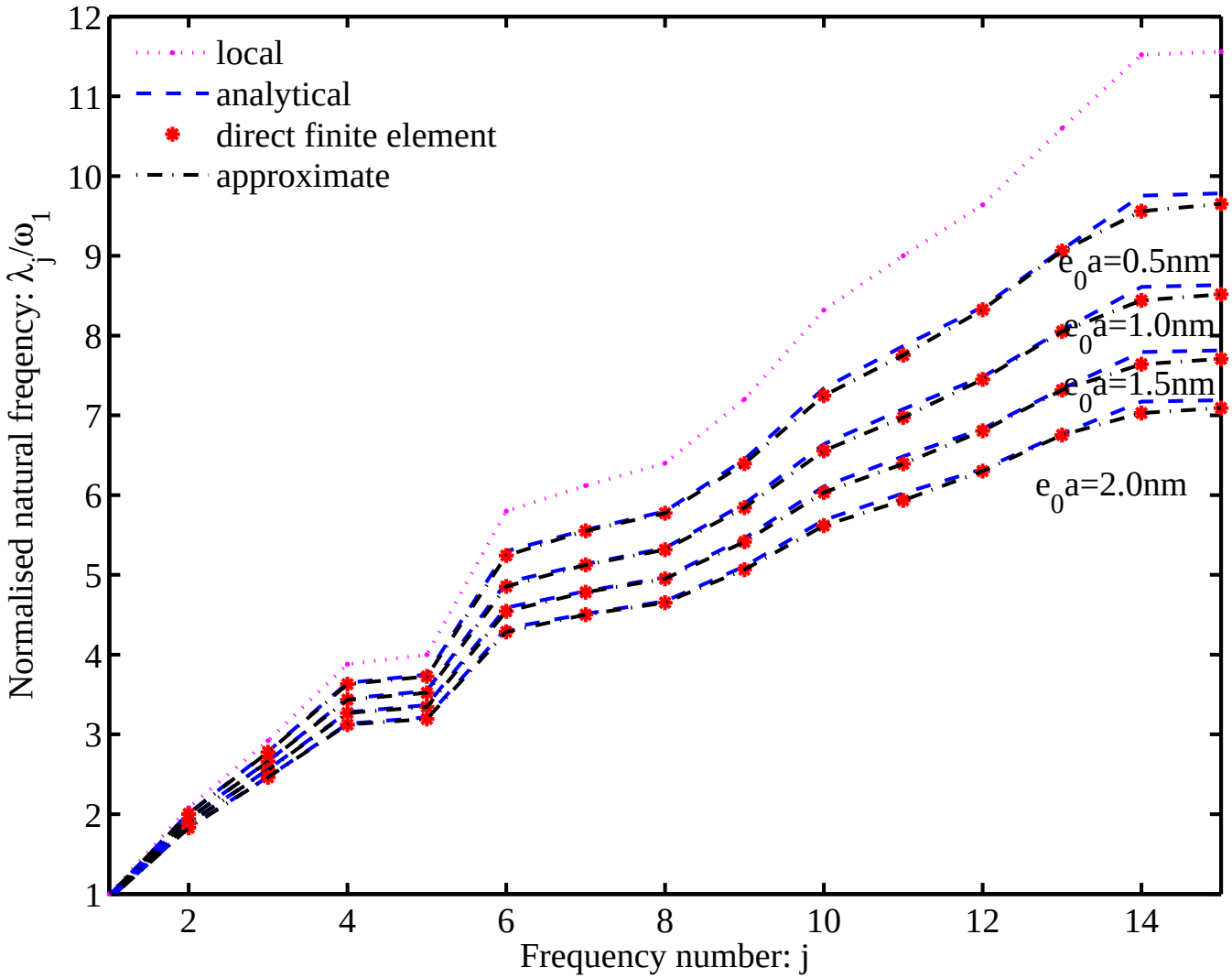
Transverse vibration of a single-layer graphene sheet

- 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

$$\lambda_{ij} = \sqrt{\frac{D}{m}} \frac{\beta_{ij}^2}{\sqrt{1 + \beta_{ij}^2 (e_0 a)^2}} \quad \text{where} \quad \beta_{ij} = \sqrt{(i\pi/L)^2 + (j\pi/W)^2}, \ i, j = 1, 2, \cdots \tag{93}$$

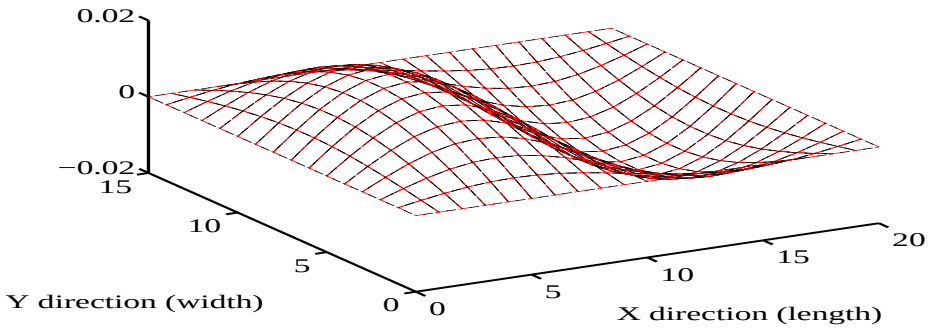
  D is the bending rigidity and m is the mass per unit area of the SLGS.
- For the finite element analysis the DWCNT is divided into 20×15 elements. The dimension of each of the system matrices become 868×868, that is $n = 868$.

Nonlocal natural frequencies of SLGS

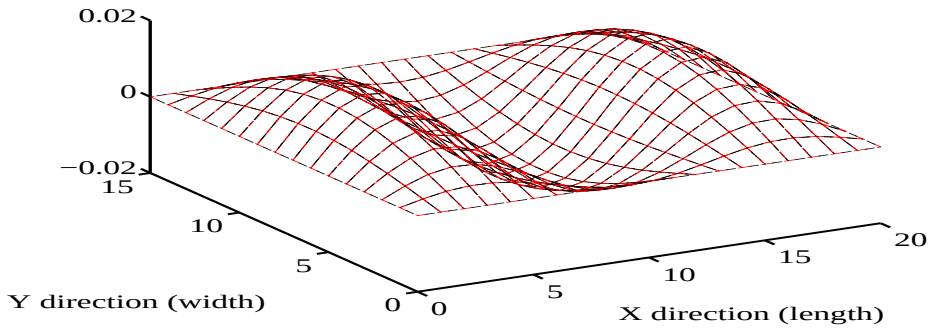


First 15 undamped natural frequencies for the transverse vibration of SLGS.

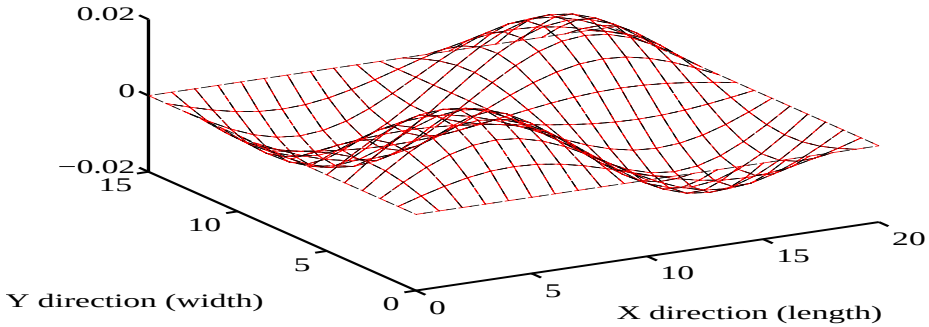
Nonlocal bending mode shapes of SLGS



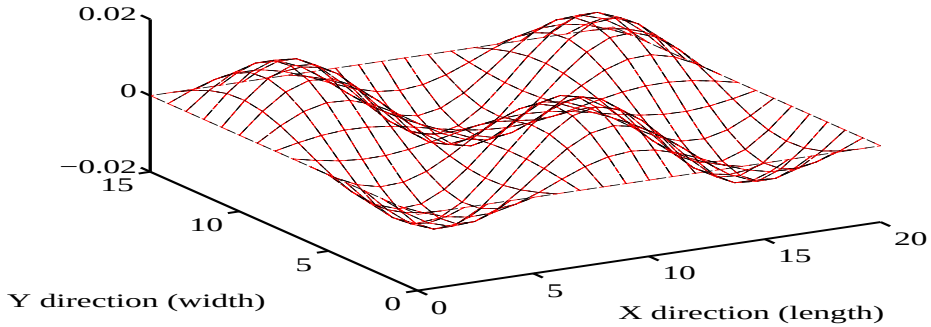
(a) Mode 2



(b) Mode 4



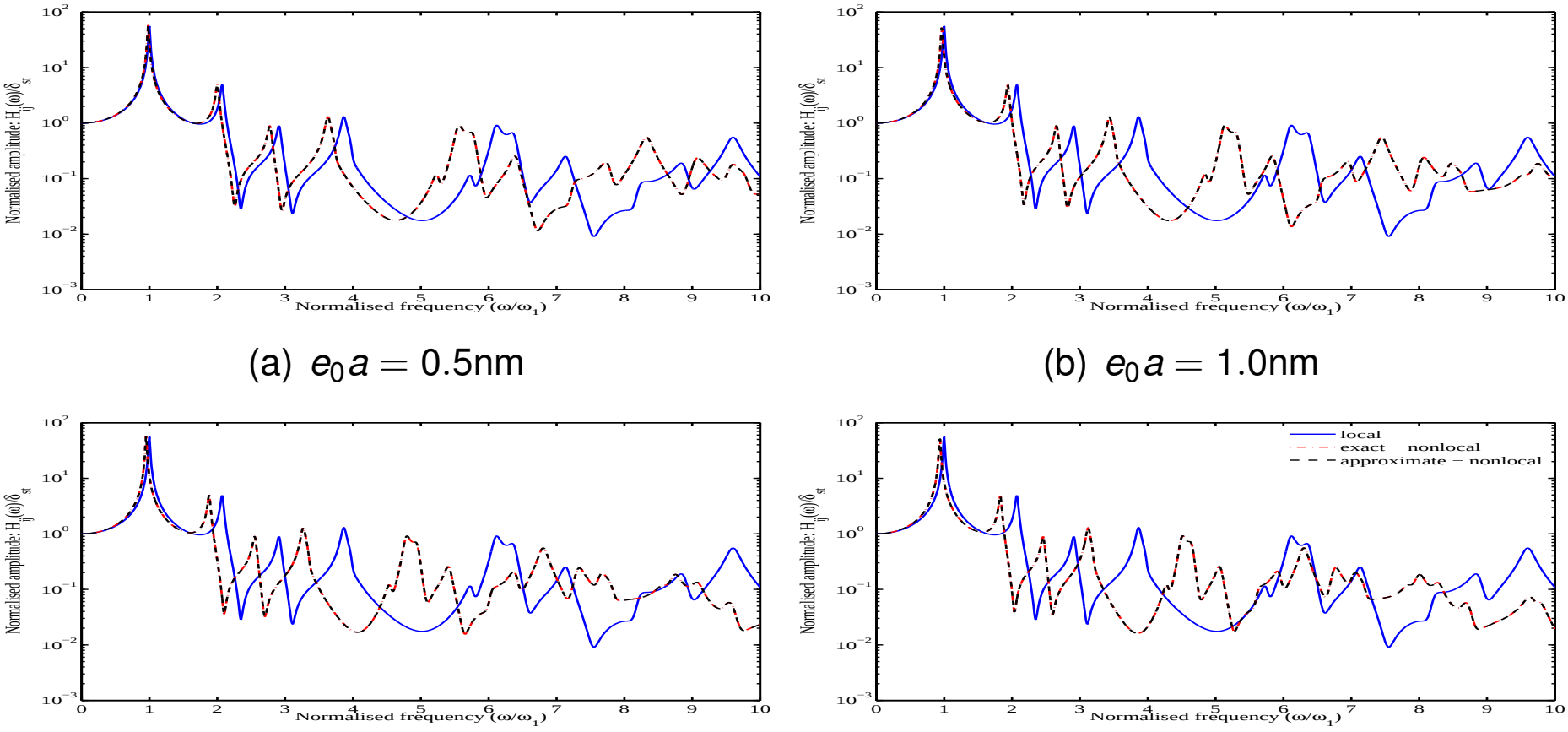
(c) Mode 5



(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).

Nonlocal frequency response of SLGS



(a) $e_0a = 0.5$nm

(b) $e_0a = 1.0$nm

(c) $e_0a = 1.5$nm

(d) $e_0a = 2.0$nm

Figure: Amplitude of the normalised frequency response $H_{ij}(\omega)$ for $i = 475, j = 342$ of the SLGS for different values of e_0a. Exact finite element results are compared with the approximate analysis based on local eigensolutions.

Conclusions

- Nonlocal elasticity is a promising theory for the modelling of nanoscale dynamical systems such as carbon nantotubes and graphene sheets.
- Equation of motion for axial vibration of nonlocal rods, bending vibration of nonlocal beams and transverse vibration of thin nonlocal plates have been described and corresponding natural frequencies are given.
- 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.

Conclusions

- 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 ω_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.

Further reading

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